wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 09:48 PM GMT

PDB ID	:	4W6R
Title	:	Crystal Structure of Full-Length Split GFP Mutant D102C Disulfide Dimer, P 1 Space Group
Authors	:	Leibly, D.J.; Waldo, G.S.; Yeates, T.O.
Deposited on	:	2014-08-20
Resolution	:	3.47 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

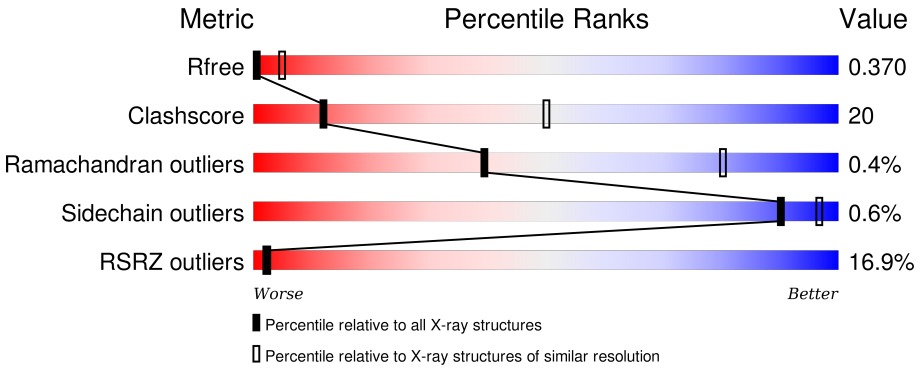
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.47 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	1173 (3.60-3.36)
Clashscore	102246	1010 (3.58-3.38)
Ramachandran outliers	100387	1245 (3.60-3.36)
Sidechain outliers	100360	1246 (3.60-3.36)
RSRZ outliers	91569	1180 (3.60-3.36)

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 <=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	234	14% 59% 31% • 8%
1	B	234	11% 58% 29% • 12%
1	C	234	15% 59% 29% 12%
1	D	234	9% 53% 28% • 17%
1	E	234	10% 66% 23% 11%

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Mol	Chain	Length	Quality of chain
1	F	234	13% 60% 24% • 14%
1	G	234	16% 51% 28% • 20%
1	H	234	17% 56% 23% • 18%
1	I	234	8% 57% 32% 11%
1	J	234	8% 51% 27% 21%
1	K	234	8% 50% 24% • 25%
1	L	234	19% 56% 28% • 16%
1	M	234	16% 50% 22% 28%
1	N	234	19% 54% 19% • 26%
1	O	234	24% 58% 32% • 9%
1	P	234	21% 64% 23% 13%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25002 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 fluorescent protein D102C.

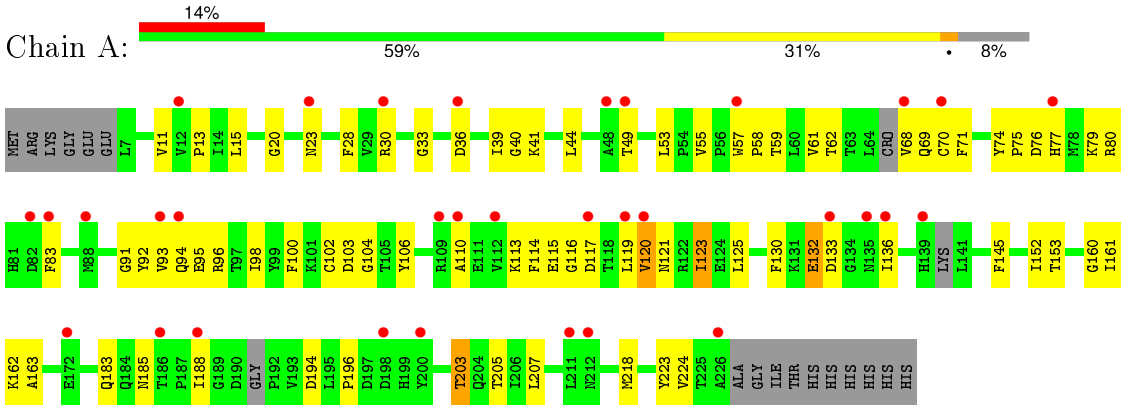
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1721	1098	291	327	5			
1	B	205	Total	C	N	O	S	0	0	0
			1649	1052	280	313	4			
1	C	207	Total	C	N	O	S	0	0	0
			1643	1052	277	309	5			
1	D	194	Total	C	N	O	S	0	0	0
			1552	993	261	293	5			
1	E	208	Total	C	N	O	S	0	0	0
			1661	1059	280	317	5			
1	F	201	Total	C	N	O	S	0	0	0
			1600	1020	270	307	3			
1	G	188	Total	C	N	O	S	0	0	0
			1497	949	262	282	4			
1	H	191	Total	C	N	O	S	0	0	0
			1537	980	264	289	4			
1	I	209	Total	C	N	O	S	0	0	0
			1671	1065	285	316	5			
1	J	184	Total	C	N	O	S	0	0	0
			1459	931	247	278	3			
1	K	175	Total	C	N	O	S	0	0	0
			1391	896	229	263	3			
1	L	197	Total	C	N	O	S	0	0	0
			1573	1002	269	298	4			
1	M	168	Total	C	N	O	S	0	0	0
			1352	864	233	251	4			
1	N	174	Total	C	N	O	S	0	0	0
			1387	876	235	273	3			
1	O	213	Total	C	N	O	S	0	0	0
			1677	1065	286	322	4			
1	P	204	Total	C	N	O	S	0	0	0
			1632	1038	281	308	5			

3 Residue-property plots (i)

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.

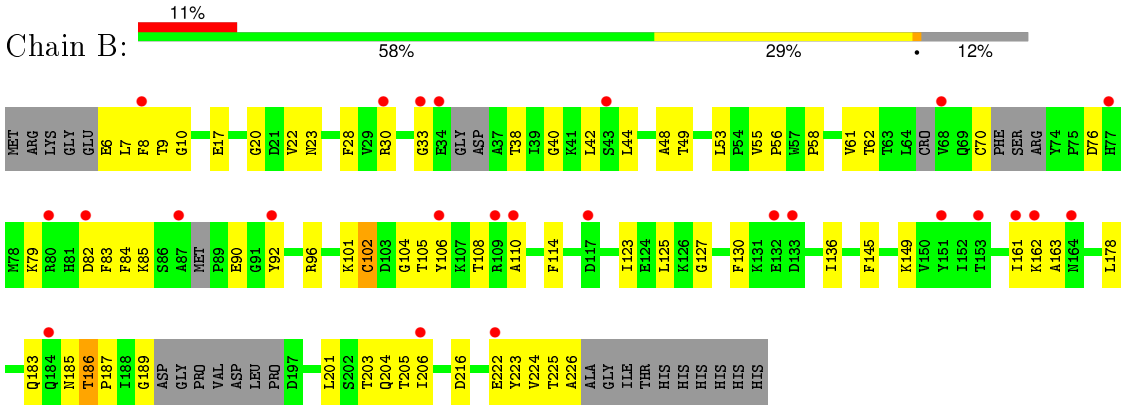
- Molecule 1: fluorescent protein D102C

Chain A:



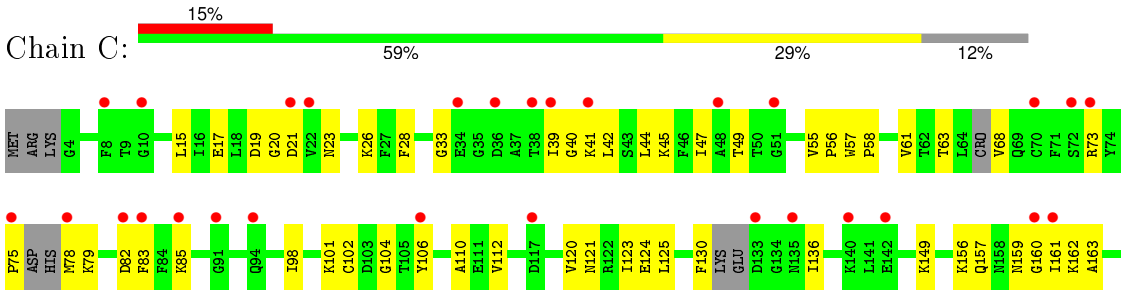
- Molecule 1: fluorescent protein D102C

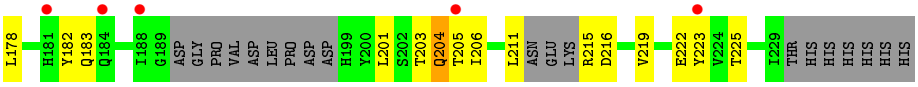
Chain B:



- Molecule 1: fluorescent protein D102C

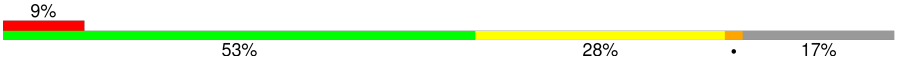
Chain C:

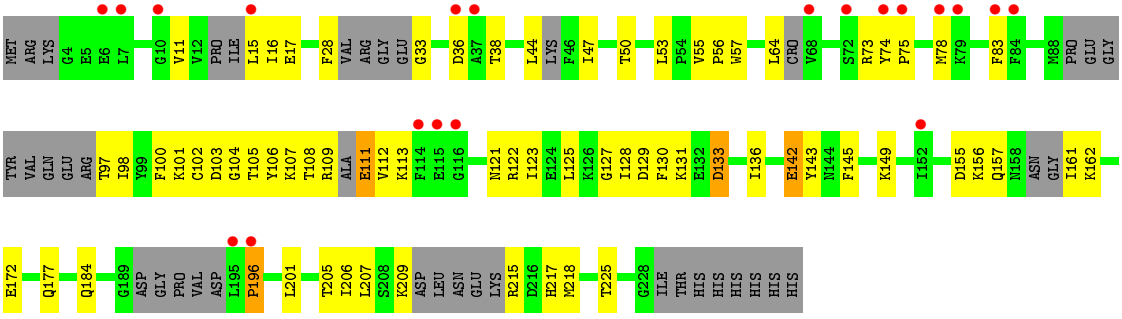




• Molecule 1: fluorescent protein D102C

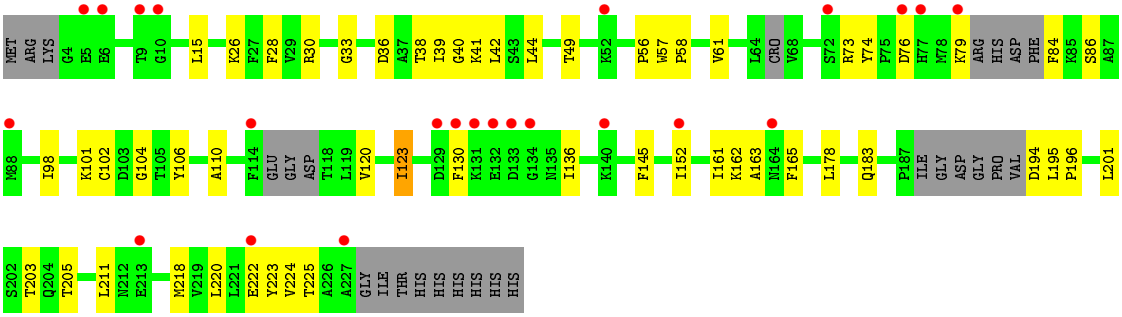
Chain D:





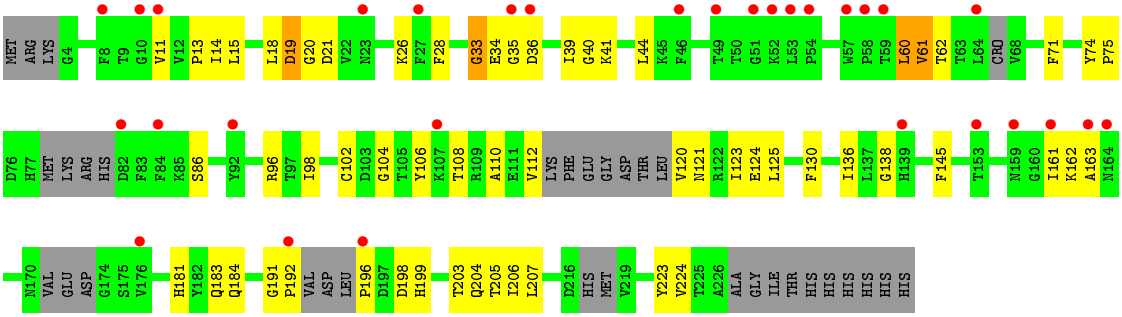
• Molecule 1: fluorescent protein D102C

Chain E:



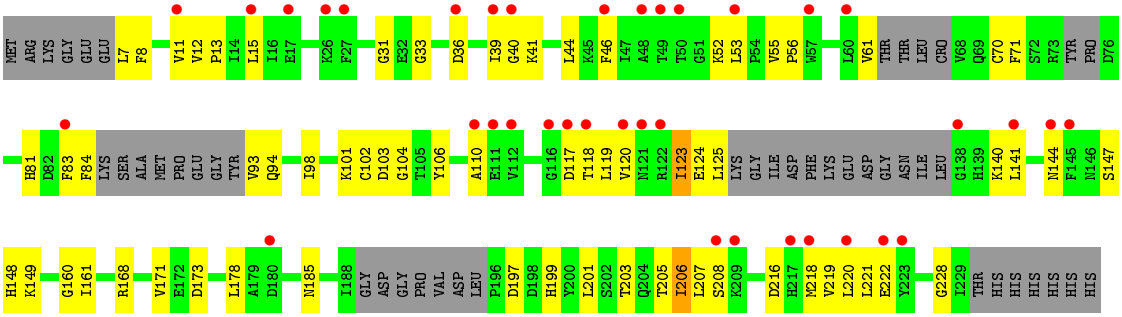
• Molecule 1: fluorescent protein D102C

Chain F:



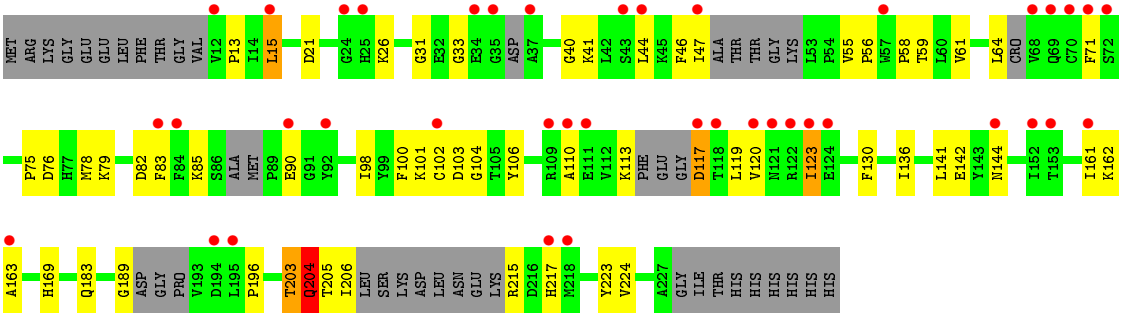
• Molecule 1: fluorescent protein D102C

Chain G:



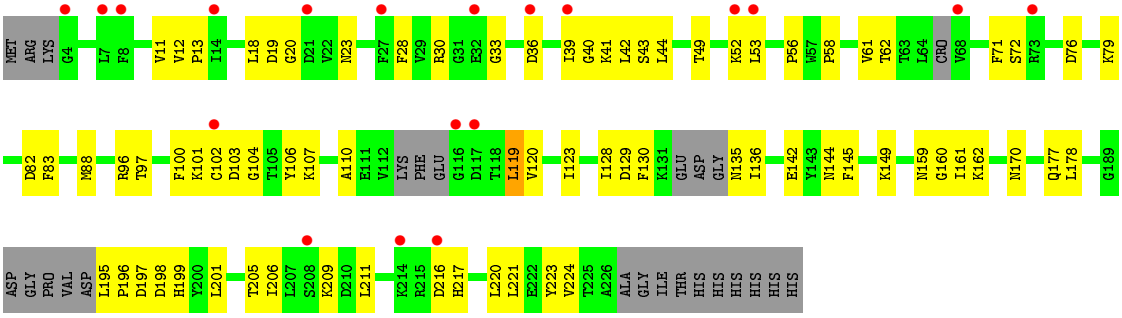
• Molecule 1: fluorescent protein D102C

Chain H:



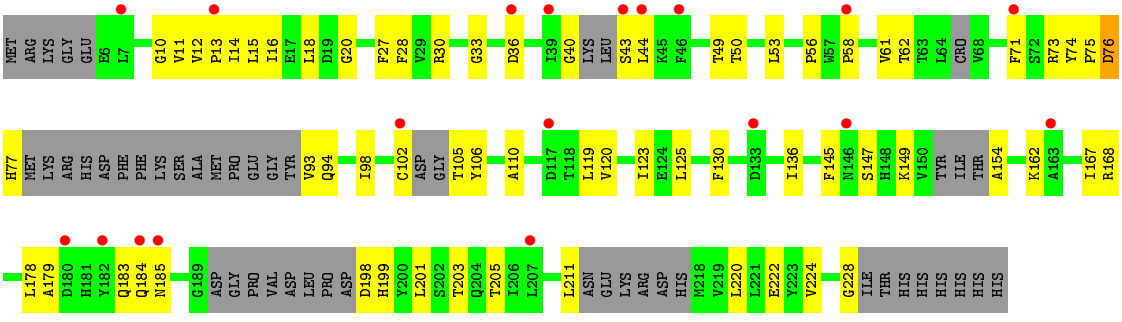
• Molecule 1: fluorescent protein D102C

Chain I:



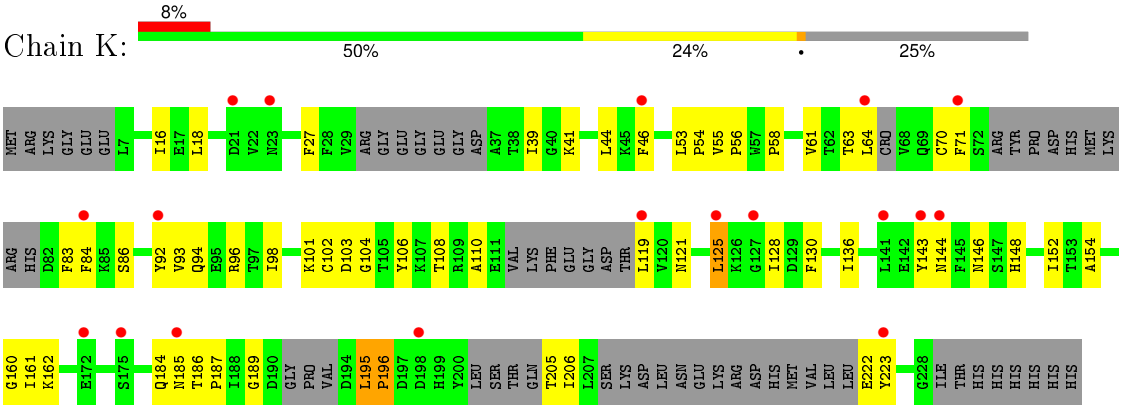
• Molecule 1: fluorescent protein D102C

Chain J:



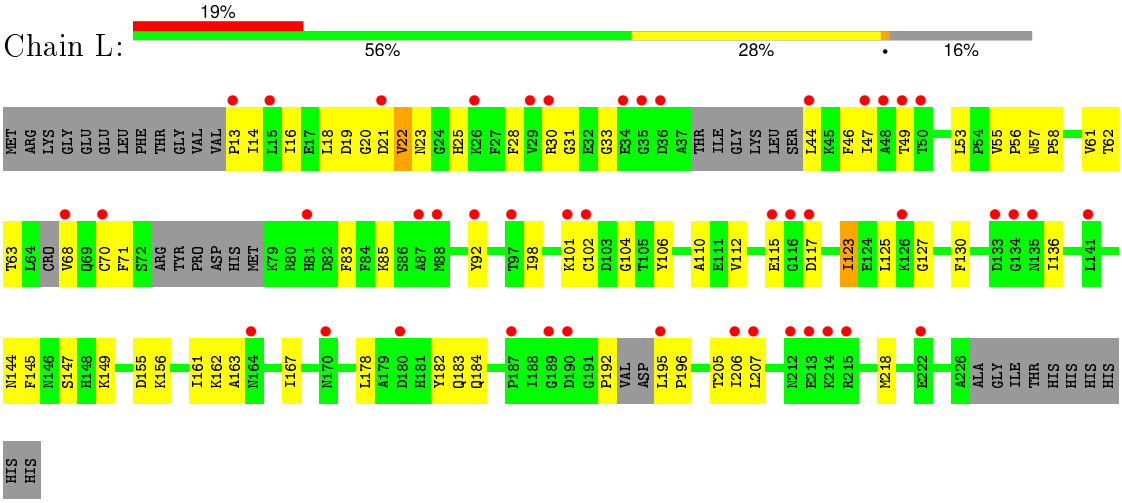
• Molecule 1: fluorescent protein D102C

Chain K:



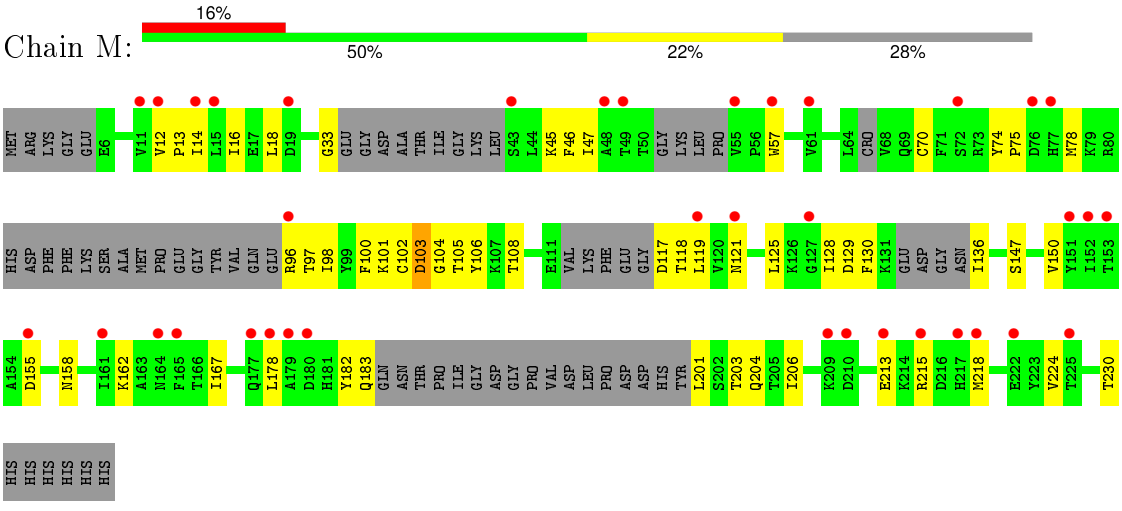
• Molecule 1: fluorescent protein D102C

Chain L:



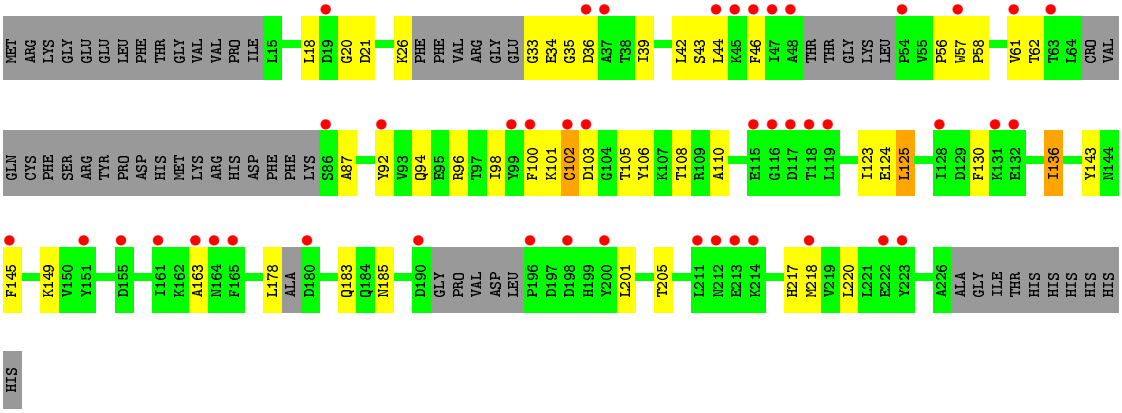
• Molecule 1: fluorescent protein D102C

Chain M:



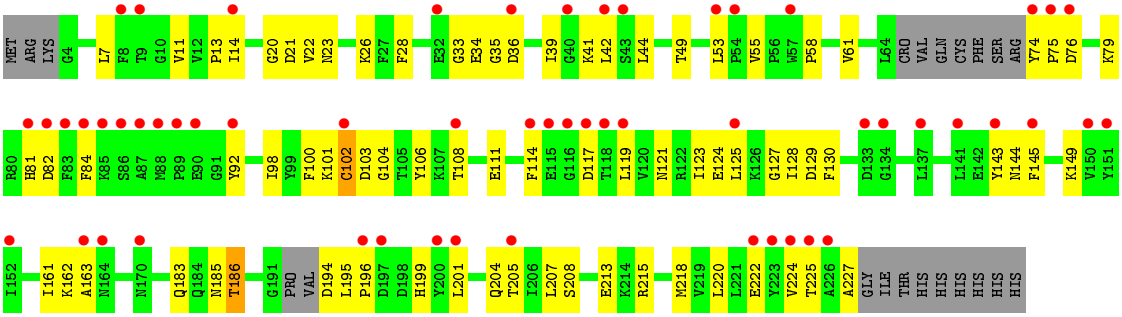
• Molecule 1: fluorescent protein D102C

Chain N:



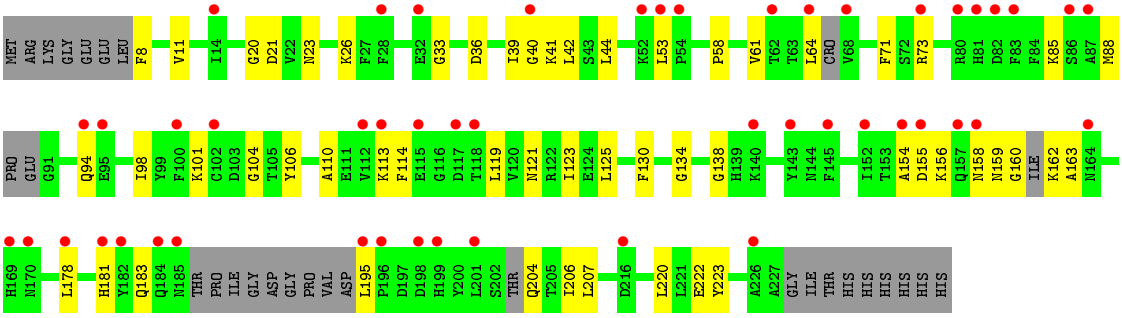
• Molecule 1: fluorescent protein D102C

Chain O:



• Molecule 1: fluorescent protein D102C

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	92.42Å 92.56Å 124.53Å 94.94° 96.17° 102.25°	Depositor
Resolution (Å)	89.88 – 3.47 89.88 – 3.47	Depositor EDS
% Data completeness (in resolution range)	89.4 (89.88-3.47) 83.9 (89.88-3.47)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 3.49Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_1555)	Depositor
R, R_{free}	0.307 , 0.357 0.326 , 0.370	Depositor DCC
R_{free} test set	4609 reflections (10.01%)	DCC
Wilson B-factor (Å^2)	101.2	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 40.0	EDS
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Outliers	0 of 46082 reflections	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	25002	wwPDB-VP
Average B, all atoms (Å^2)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.375 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	0.38	0/1758	0.82	3/2375 (0.1%)
1	B	0.34	0/1681	0.77	1/2265 (0.0%)
1	C	0.33	0/1675	0.80	1/2258 (0.0%)
1	D	0.38	0/1579	0.89	3/2121 (0.1%)
1	E	0.33	0/1694	0.78	4/2287 (0.2%)
1	F	0.36	0/1631	0.81	2/2199 (0.1%)
1	G	0.35	0/1524	0.82	0/2053
1	H	0.34	0/1567	0.82	4/2112 (0.2%)
1	I	0.35	0/1705	0.84	4/2302 (0.2%)
1	J	0.35	0/1483	0.82	0/1998
1	K	0.41	0/1417	0.81	2/1912 (0.1%)
1	L	0.33	0/1605	0.76	1/2164 (0.0%)
1	M	0.31	0/1373	0.84	0/1847
1	N	0.33	0/1410	0.86	3/1899 (0.2%)
1	O	0.40	0/1712	0.81	1/2314 (0.0%)
1	P	0.33	0/1663	0.79	1/2239 (0.0%)
All	All	0.35	0/25477	0.81	30/34345 (0.1%)

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	D	0	1

There are no bond length outliers.

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	15	LEU	CA-CB-CG	7.89	133.45	115.30
1	D	125	LEU	CA-CB-CG	7.63	132.85	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	220	LEU	CA-CB-CG	7.57	132.72	115.30
1	A	203	THR	N-CA-C	7.12	130.21	111.00
1	H	203	THR	N-CA-C	6.86	129.52	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	111	GLU	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	1721	0	1680	100	0
1	B	1649	0	1615	84	0
1	C	1643	0	1611	59	1
1	D	1552	0	1511	61	1
1	E	1661	0	1623	38	0
1	F	1600	0	1557	47	1
1	G	1497	0	1460	86	0
1	H	1537	0	1487	56	0
1	I	1671	0	1633	95	0
1	J	1459	0	1431	58	1
1	K	1391	0	1359	51	0
1	L	1573	0	1532	60	0
1	M	1352	0	1339	46	0
1	N	1387	0	1351	40	0
1	O	1677	0	1616	102	0
1	P	1632	0	1586	42	0
All	All	25002	0	24391	986	2

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 20.

The worst 5 of 986 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:I:28:PHE:CE2	1:I:30:ARG:HG3	1.44	1.51
1:A:152:ILE:O	1:A:153:THR:HG22	1.19	1.34
1:D:15:LEU:O	1:D:15:LEU:HD12	1.31	1.30
1:B:106:TYR:CE1	1:B:130:PHE:CE1	2.24	1.24
1:G:44:LEU:O	1:G:219:VAL:HG13	1.36	1.24

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:GLN:OE1	1:F:184:GLN:NE2[1_445]	2.14	0.06
1:C:17:GLU:OE2	1:J:50:THR:OG1[1_455]	2.17	0.03

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	207/234 (88%)	195 (94%)	11 (5%)	1 (0%)	34	77
1	B	193/234 (82%)	184 (95%)	8 (4%)	1 (0%)	34	77
1	C	195/234 (83%)	188 (96%)	6 (3%)	1 (0%)	34	77
1	D	174/234 (74%)	161 (92%)	12 (7%)	1 (1%)	30	74
1	E	198/234 (85%)	191 (96%)	6 (3%)	1 (0%)	34	77
1	F	187/234 (80%)	180 (96%)	6 (3%)	1 (0%)	34	77
1	G	176/234 (75%)	167 (95%)	8 (4%)	1 (1%)	30	74
1	H	175/234 (75%)	169 (97%)	6 (3%)	0	100	100
1	I	199/234 (85%)	192 (96%)	6 (3%)	1 (0%)	34	77
1	J	168/234 (72%)	163 (97%)	5 (3%)	0	100	100
1	K	159/234 (68%)	154 (97%)	4 (2%)	1 (1%)	30	74
1	L	187/234 (80%)	181 (97%)	5 (3%)	1 (0%)	34	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	M	152/234 (65%)	149 (98%)	2 (1%)	1 (1%)	26 72
1	N	162/234 (69%)	159 (98%)	3 (2%)	0	100 100
1	O	207/234 (88%)	198 (96%)	7 (3%)	2 (1%)	19 65
1	P	192/234 (82%)	186 (97%)	6 (3%)	0	100 100
All	All	2931/3744 (78%)	2817 (96%)	101 (3%)	13 (0%)	39 80

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	VAL
1	F	61	VAL
1	G	206	ILE
1	D	196	PRO
1	C	204	GLN

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	189/204 (93%)	188 (100%)	1 (0%)	92 97
1	B	181/204 (89%)	180 (99%)	1 (1%)	90 97
1	C	178/204 (87%)	177 (99%)	1 (1%)	90 97
1	D	170/204 (83%)	170 (100%)	0	100 100
1	E	182/204 (89%)	181 (100%)	1 (0%)	92 97
1	F	175/204 (86%)	174 (99%)	1 (1%)	90 97
1	G	163/204 (80%)	162 (99%)	1 (1%)	90 97
1	H	168/204 (82%)	166 (99%)	2 (1%)	78 91
1	I	183/204 (90%)	181 (99%)	2 (1%)	80 92
1	J	160/204 (78%)	159 (99%)	1 (1%)	90 97
1	K	152/204 (74%)	151 (99%)	1 (1%)	88 95
1	L	171/204 (84%)	170 (99%)	1 (1%)	90 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	149/204 (73%)	148 (99%)	1 (1%)	88 95
1	N	153/204 (75%)	152 (99%)	1 (1%)	88 95
1	O	179/204 (88%)	178 (99%)	1 (1%)	90 97
1	P	177/204 (87%)	177 (100%)	0	100 100
All	All	2730/3264 (84%)	2714 (99%)	16 (1%)	90 97

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	204	GLN
1	I	119	LEU
1	L	123	ILE
1	H	123	ILE
1	M	121	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	183	GLN
1	K	144	ASN
1	N	164	ASN
1	H	94	GLN
1	I	135	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 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, 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	215/234 (91%)	1.01	33 (15%)	3	3	50, 80, 148, 324	0
1	B	205/234 (87%)	0.78	25 (12%)	5	6	51, 87, 175, 274	0
1	C	207/234 (88%)	0.93	34 (16%)	2	2	55, 91, 164, 338	0
1	D	194/234 (82%)	0.62	20 (10%)	9	8	57, 92, 169, 237	0
1	E	208/234 (88%)	0.70	23 (11%)	7	7	64, 96, 157, 204	0
1	F	201/234 (85%)	0.94	30 (14%)	3	3	69, 106, 174, 357	0
1	G	188/234 (80%)	0.98	37 (19%)	1	2	52, 103, 181, 284	0
1	H	191/234 (81%)	1.13	40 (20%)	1	1	69, 102, 172, 382	0
1	I	209/234 (89%)	0.68	19 (9%)	11	10	64, 98, 165, 249	0
1	J	184/234 (78%)	0.63	19 (10%)	9	8	51, 95, 166, 270	0
1	K	175/234 (74%)	0.68	18 (10%)	9	8	73, 102, 181, 323	0
1	L	197/234 (84%)	1.19	45 (22%)	1	1	67, 114, 206, 293	0
1	M	168/234 (71%)	1.30	37 (22%)	1	1	75, 119, 203, 375	0
1	N	174/234 (74%)	1.27	45 (25%)	1	1	72, 130, 219, 388	0
1	O	213/234 (91%)	1.53	56 (26%)	1	1	54, 126, 205, 302	0
1	P	204/234 (87%)	1.25	49 (24%)	1	1	73, 134, 217, 464	0
All	All	3133/3744 (83%)	0.98	530 (16%)	2	2	50, 104, 188, 464	0

The worst 5 of 530 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	164	ASN	11.6
1	M	164	ASN	9.9
1	O	86	SER	9.4
1	M	76	ASP	9.2
1	O	223	TYR	9.0

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.