wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 08:27 PM EDT

PDB ID	:	5U9O
Title	:	Cocrystal structure of the intermembrane space region of the plastid division proteins PARC6 and PDV1
Authors	:	Delmar, J.A.; Chou, T.H.
Deposited on	:	2016-12-16
Resolution	:	3.37 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:

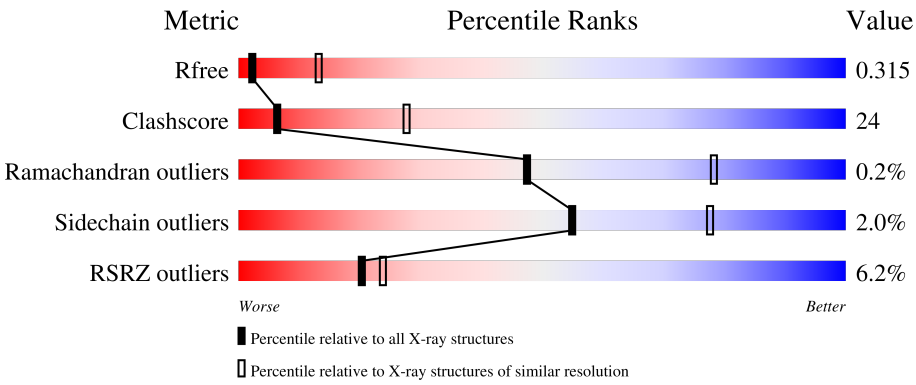
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.37 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	1691 (3.46-3.30)
Clashscore	141614	1762 (3.46-3.30)
Ramachandran outliers	138981	1732 (3.46-3.30)
Sidechain outliers	138945	1731 (3.46-3.30)
RSRZ outliers	127900	1635 (3.46-3.30)

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 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	187	6%, 34%, 41%, •, 22%
1	B	187	3%, 38%, 38%, •, 23%
1	C	187	2%, 39%, 37%, •, 22%
1	D	187	5%, 40%, 37%, •, 22%
1	E	187	5%, 44%, 32%, •, 23%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	187	6% 45% 30% • 24%
1	G	187	8% 37% 36% • 26%
1	H	187	3% 37% 37% • 25%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9299 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 Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	145	1174	745	195	228	6	0	0	0
1	B	144	1173	745	195	227	6	0	0	0
1	C	145	1178	747	195	230	6	0	0	0
1	D	146	1188	755	196	231	6	0	0	0
1	E	144	1170	744	192	228	6	0	0	0
1	F	142	1156	734	192	224	6	0	0	0
1	G	139	1127	716	184	221	6	0	0	0
1	H	140	1133	721	183	223	6	0	0	0

There are 208 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	670	MET	-	initiating methionine	UNP Q8VY16
A	671	GLY	-	expression tag	UNP Q8VY16
A	672	HIS	-	expression tag	UNP Q8VY16
A	673	HIS	-	expression tag	UNP Q8VY16
A	674	HIS	-	expression tag	UNP Q8VY16
A	675	HIS	-	expression tag	UNP Q8VY16
A	676	HIS	-	expression tag	UNP Q8VY16
A	677	HIS	-	expression tag	UNP Q8VY16
A	678	LEU	-	expression tag	UNP Q8VY16
A	679	VAL	-	expression tag	UNP Q8VY16
A	680	PRO	-	expression tag	UNP Q8VY16
A	681	ARG	-	expression tag	UNP Q8VY16

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	682	GLY	-	expression tag	UNP Q8VY16
A	683	SER	-	expression tag	UNP Q8VY16
A	820	GLY	-	linker	UNP Q8VY16
A	821	SER	-	linker	UNP Q8VY16
A	822	GLY	-	linker	UNP Q8VY16
A	823	SER	-	linker	UNP Q8VY16
A	824	GLY	-	linker	UNP Q8VY16
A	825	SER	-	linker	UNP Q8VY16
A	826	GLY	-	linker	UNP Q8VY16
A	827	SER	-	linker	UNP Q8VY16
A	828	GLY	-	linker	UNP Q8VY16
A	829	SER	-	linker	UNP Q8VY16
A	830	GLY	-	linker	UNP Q8VY16
A	831	SER	-	linker	UNP Q8VY16
B	670	MET	-	initiating methionine	UNP Q8VY16
B	671	GLY	-	expression tag	UNP Q8VY16
B	672	HIS	-	expression tag	UNP Q8VY16
B	673	HIS	-	expression tag	UNP Q8VY16
B	674	HIS	-	expression tag	UNP Q8VY16
B	675	HIS	-	expression tag	UNP Q8VY16
B	676	HIS	-	expression tag	UNP Q8VY16
B	677	HIS	-	expression tag	UNP Q8VY16
B	678	LEU	-	expression tag	UNP Q8VY16
B	679	VAL	-	expression tag	UNP Q8VY16
B	680	PRO	-	expression tag	UNP Q8VY16
B	681	ARG	-	expression tag	UNP Q8VY16
B	682	GLY	-	expression tag	UNP Q8VY16
B	683	SER	-	expression tag	UNP Q8VY16
B	820	GLY	-	linker	UNP Q8VY16
B	821	SER	-	linker	UNP Q8VY16
B	822	GLY	-	linker	UNP Q8VY16
B	823	SER	-	linker	UNP Q8VY16
B	824	GLY	-	linker	UNP Q8VY16
B	825	SER	-	linker	UNP Q8VY16
B	826	GLY	-	linker	UNP Q8VY16
B	827	SER	-	linker	UNP Q8VY16
B	828	GLY	-	linker	UNP Q8VY16
B	829	SER	-	linker	UNP Q8VY16
B	830	GLY	-	linker	UNP Q8VY16
B	831	SER	-	linker	UNP Q8VY16
C	670	MET	-	initiating methionine	UNP Q8VY16
C	671	GLY	-	expression tag	UNP Q8VY16

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	672	HIS	-	expression tag	UNP Q8VY16
C	673	HIS	-	expression tag	UNP Q8VY16
C	674	HIS	-	expression tag	UNP Q8VY16
C	675	HIS	-	expression tag	UNP Q8VY16
C	676	HIS	-	expression tag	UNP Q8VY16
C	677	HIS	-	expression tag	UNP Q8VY16
C	678	LEU	-	expression tag	UNP Q8VY16
C	679	VAL	-	expression tag	UNP Q8VY16
C	680	PRO	-	expression tag	UNP Q8VY16
C	681	ARG	-	expression tag	UNP Q8VY16
C	682	GLY	-	expression tag	UNP Q8VY16
C	683	SER	-	expression tag	UNP Q8VY16
C	820	GLY	-	linker	UNP Q8VY16
C	821	SER	-	linker	UNP Q8VY16
C	822	GLY	-	linker	UNP Q8VY16
C	823	SER	-	linker	UNP Q8VY16
C	824	GLY	-	linker	UNP Q8VY16
C	825	SER	-	linker	UNP Q8VY16
C	826	GLY	-	linker	UNP Q8VY16
C	827	SER	-	linker	UNP Q8VY16
C	828	GLY	-	linker	UNP Q8VY16
C	829	SER	-	linker	UNP Q8VY16
C	830	GLY	-	linker	UNP Q8VY16
C	831	SER	-	linker	UNP Q8VY16
D	670	MET	-	initiating methionine	UNP Q8VY16
D	671	GLY	-	expression tag	UNP Q8VY16
D	672	HIS	-	expression tag	UNP Q8VY16
D	673	HIS	-	expression tag	UNP Q8VY16
D	674	HIS	-	expression tag	UNP Q8VY16
D	675	HIS	-	expression tag	UNP Q8VY16
D	676	HIS	-	expression tag	UNP Q8VY16
D	677	HIS	-	expression tag	UNP Q8VY16
D	678	LEU	-	expression tag	UNP Q8VY16
D	679	VAL	-	expression tag	UNP Q8VY16
D	680	PRO	-	expression tag	UNP Q8VY16
D	681	ARG	-	expression tag	UNP Q8VY16
D	682	GLY	-	expression tag	UNP Q8VY16
D	683	SER	-	expression tag	UNP Q8VY16
D	820	GLY	-	linker	UNP Q8VY16
D	821	SER	-	linker	UNP Q8VY16
D	822	GLY	-	linker	UNP Q8VY16
D	823	SER	-	linker	UNP Q8VY16

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	824	GLY	-	linker	UNP Q8VY16
D	825	SER	-	linker	UNP Q8VY16
D	826	GLY	-	linker	UNP Q8VY16
D	827	SER	-	linker	UNP Q8VY16
D	828	GLY	-	linker	UNP Q8VY16
D	829	SER	-	linker	UNP Q8VY16
D	830	GLY	-	linker	UNP Q8VY16
D	831	SER	-	linker	UNP Q8VY16
E	670	MET	-	initiating methionine	UNP Q8VY16
E	671	GLY	-	expression tag	UNP Q8VY16
E	672	HIS	-	expression tag	UNP Q8VY16
E	673	HIS	-	expression tag	UNP Q8VY16
E	674	HIS	-	expression tag	UNP Q8VY16
E	675	HIS	-	expression tag	UNP Q8VY16
E	676	HIS	-	expression tag	UNP Q8VY16
E	677	HIS	-	expression tag	UNP Q8VY16
E	678	LEU	-	expression tag	UNP Q8VY16
E	679	VAL	-	expression tag	UNP Q8VY16
E	680	PRO	-	expression tag	UNP Q8VY16
E	681	ARG	-	expression tag	UNP Q8VY16
E	682	GLY	-	expression tag	UNP Q8VY16
E	683	SER	-	expression tag	UNP Q8VY16
E	820	GLY	-	linker	UNP Q8VY16
E	821	SER	-	linker	UNP Q8VY16
E	822	GLY	-	linker	UNP Q8VY16
E	823	SER	-	linker	UNP Q8VY16
E	824	GLY	-	linker	UNP Q8VY16
E	825	SER	-	linker	UNP Q8VY16
E	826	GLY	-	linker	UNP Q8VY16
E	827	SER	-	linker	UNP Q8VY16
E	828	GLY	-	linker	UNP Q8VY16
E	829	SER	-	linker	UNP Q8VY16
E	830	GLY	-	linker	UNP Q8VY16
E	831	SER	-	linker	UNP Q8VY16
F	670	MET	-	initiating methionine	UNP Q8VY16
F	671	GLY	-	expression tag	UNP Q8VY16
F	672	HIS	-	expression tag	UNP Q8VY16
F	673	HIS	-	expression tag	UNP Q8VY16
F	674	HIS	-	expression tag	UNP Q8VY16
F	675	HIS	-	expression tag	UNP Q8VY16
F	676	HIS	-	expression tag	UNP Q8VY16
F	677	HIS	-	expression tag	UNP Q8VY16

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	678	LEU	-	expression tag	UNP Q8VY16
F	679	VAL	-	expression tag	UNP Q8VY16
F	680	PRO	-	expression tag	UNP Q8VY16
F	681	ARG	-	expression tag	UNP Q8VY16
F	682	GLY	-	expression tag	UNP Q8VY16
F	683	SER	-	expression tag	UNP Q8VY16
F	820	GLY	-	linker	UNP Q8VY16
F	821	SER	-	linker	UNP Q8VY16
F	822	GLY	-	linker	UNP Q8VY16
F	823	SER	-	linker	UNP Q8VY16
F	824	GLY	-	linker	UNP Q8VY16
F	825	SER	-	linker	UNP Q8VY16
F	826	GLY	-	linker	UNP Q8VY16
F	827	SER	-	linker	UNP Q8VY16
F	828	GLY	-	linker	UNP Q8VY16
F	829	SER	-	linker	UNP Q8VY16
F	830	GLY	-	linker	UNP Q8VY16
F	831	SER	-	linker	UNP Q8VY16
G	670	MET	-	initiating methionine	UNP Q8VY16
G	671	GLY	-	expression tag	UNP Q8VY16
G	672	HIS	-	expression tag	UNP Q8VY16
G	673	HIS	-	expression tag	UNP Q8VY16
G	674	HIS	-	expression tag	UNP Q8VY16
G	675	HIS	-	expression tag	UNP Q8VY16
G	676	HIS	-	expression tag	UNP Q8VY16
G	677	HIS	-	expression tag	UNP Q8VY16
G	678	LEU	-	expression tag	UNP Q8VY16
G	679	VAL	-	expression tag	UNP Q8VY16
G	680	PRO	-	expression tag	UNP Q8VY16
G	681	ARG	-	expression tag	UNP Q8VY16
G	682	GLY	-	expression tag	UNP Q8VY16
G	683	SER	-	expression tag	UNP Q8VY16
G	820	GLY	-	linker	UNP Q8VY16
G	821	SER	-	linker	UNP Q8VY16
G	822	GLY	-	linker	UNP Q8VY16
G	823	SER	-	linker	UNP Q8VY16
G	824	GLY	-	linker	UNP Q8VY16
G	825	SER	-	linker	UNP Q8VY16
G	826	GLY	-	linker	UNP Q8VY16
G	827	SER	-	linker	UNP Q8VY16
G	828	GLY	-	linker	UNP Q8VY16
G	829	SER	-	linker	UNP Q8VY16

Continued on next page...

Continued from previous page...

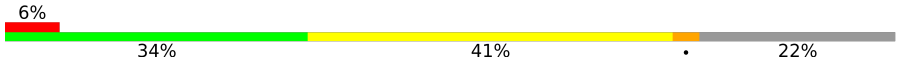
Chain	Residue	Modelled	Actual	Comment	Reference
G	830	GLY	-	linker	UNP Q8VY16
G	831	SER	-	linker	UNP Q8VY16
H	670	MET	-	initiating methionine	UNP Q8VY16
H	671	GLY	-	expression tag	UNP Q8VY16
H	672	HIS	-	expression tag	UNP Q8VY16
H	673	HIS	-	expression tag	UNP Q8VY16
H	674	HIS	-	expression tag	UNP Q8VY16
H	675	HIS	-	expression tag	UNP Q8VY16
H	676	HIS	-	expression tag	UNP Q8VY16
H	677	HIS	-	expression tag	UNP Q8VY16
H	678	LEU	-	expression tag	UNP Q8VY16
H	679	VAL	-	expression tag	UNP Q8VY16
H	680	PRO	-	expression tag	UNP Q8VY16
H	681	ARG	-	expression tag	UNP Q8VY16
H	682	GLY	-	expression tag	UNP Q8VY16
H	683	SER	-	expression tag	UNP Q8VY16
H	820	GLY	-	linker	UNP Q8VY16
H	821	SER	-	linker	UNP Q8VY16
H	822	GLY	-	linker	UNP Q8VY16
H	823	SER	-	linker	UNP Q8VY16
H	824	GLY	-	linker	UNP Q8VY16
H	825	SER	-	linker	UNP Q8VY16
H	826	GLY	-	linker	UNP Q8VY16
H	827	SER	-	linker	UNP Q8VY16
H	828	GLY	-	linker	UNP Q8VY16
H	829	SER	-	linker	UNP Q8VY16
H	830	GLY	-	linker	UNP Q8VY16
H	831	SER	-	linker	UNP Q8VY16

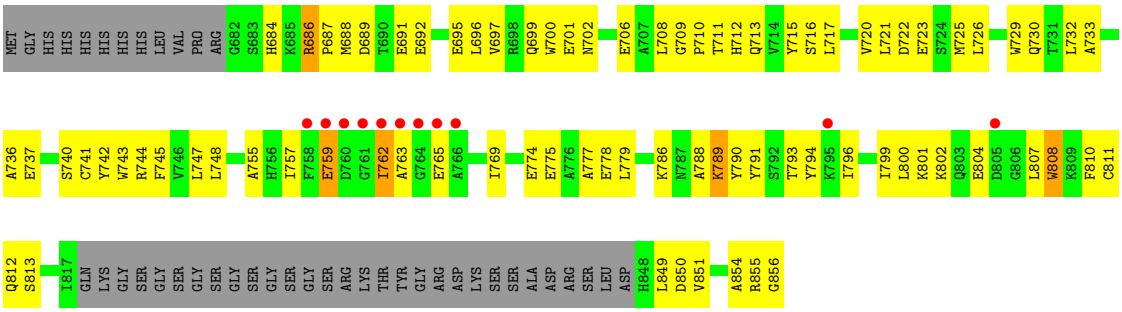
3 Residue-property plots (i)

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: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

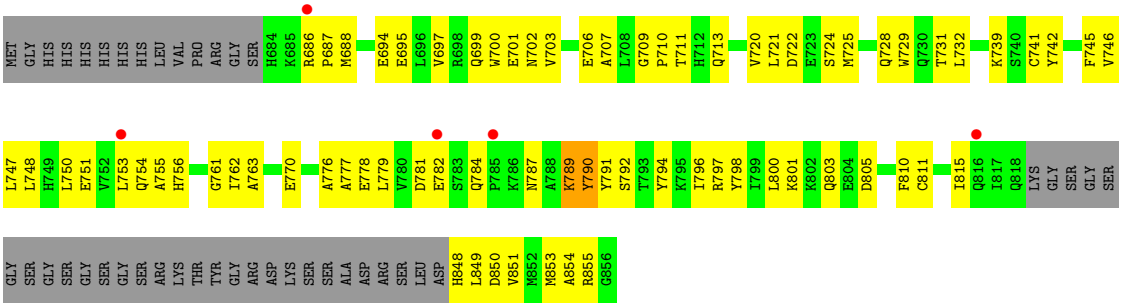
Chain A:





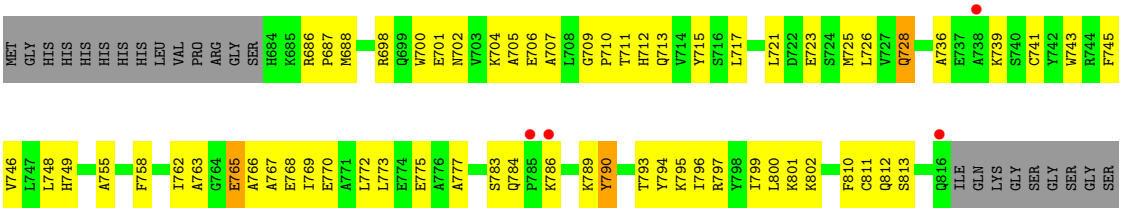
• Molecule 1: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

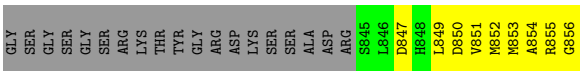
Chain B:



• Molecule 1: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

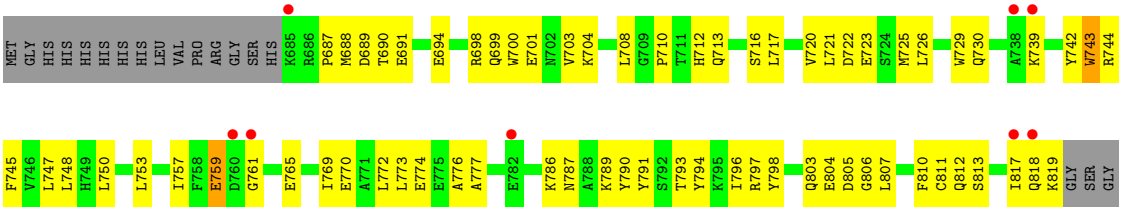
Chain C:

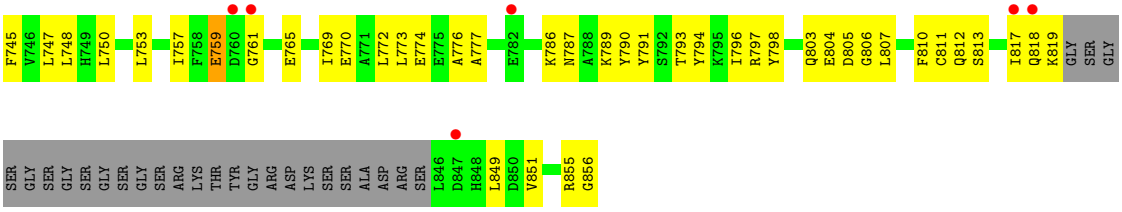




• Molecule 1: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

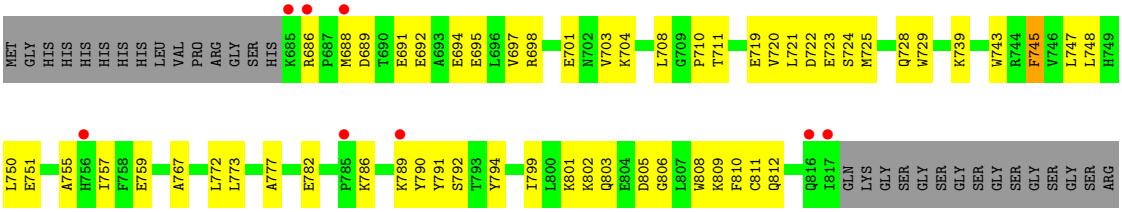
Chain D:





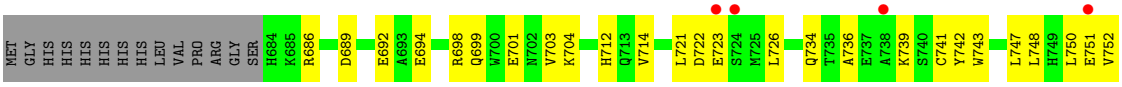
• Molecule 1: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

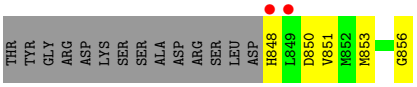
Chain E:



• Molecule 1: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

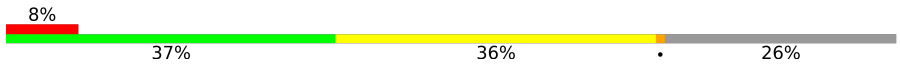
Chain F:

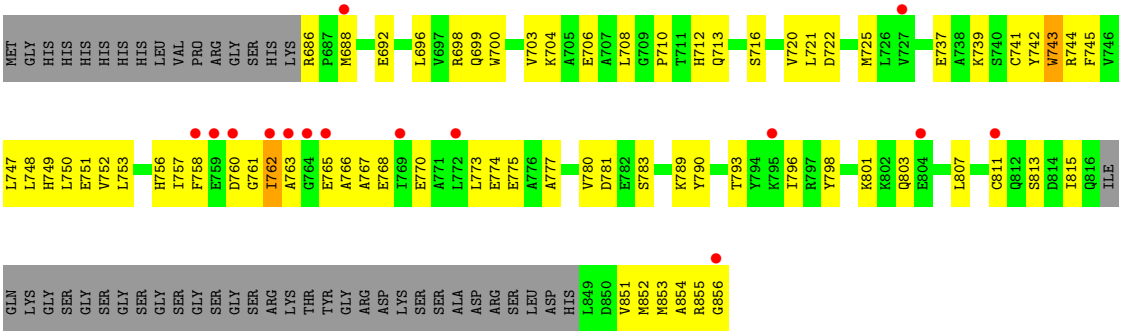




• Molecule 1: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

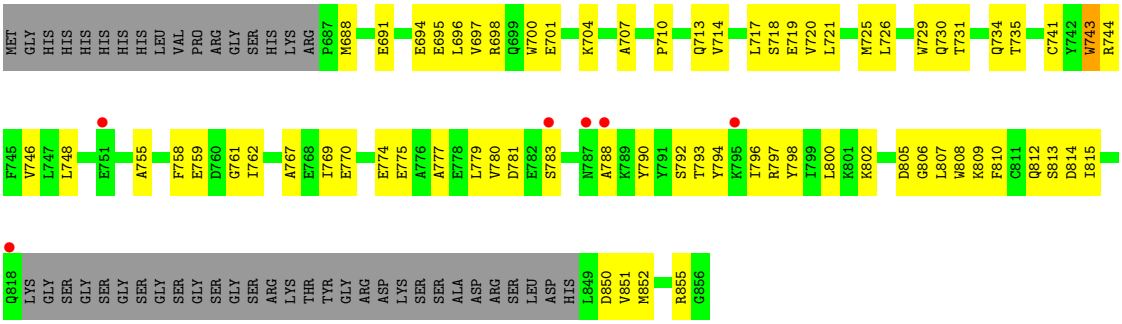
Chain G:





• Molecule 1: Plastid division protein CDP1, chloroplastic,Plastid division protein PDV1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.23Å 80.19Å 84.07Å 88.36° 80.99° 83.49°	Depositor
Resolution (Å)	38.23 – 3.37 38.23 – 3.37	Depositor EDS
% Data completeness (in resolution range)	97.7 (38.23-3.37) 97.8 (38.23-3.37)	Depositor EDS
R_{merge}	0.29	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.29 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155, Coot	Depositor
R, R_{free}	0.250 , 0.318 0.248 , 0.315	Depositor DCC
R_{free} test set	1028 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å^2)	54.1	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	9299	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.65% 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	0.40	0/1197	0.64	1/1617 (0.1%)
1	B	0.35	0/1196	0.59	0/1616
1	C	0.44	0/1201	0.57	0/1623
1	D	0.37	0/1210	0.58	0/1634
1	E	0.38	1/1192 (0.1%)	0.55	0/1611
1	F	0.31	0/1179	0.52	0/1593
1	G	0.33	0/1148	0.58	0/1552
1	H	0.34	0/1154	0.53	0/1560
All	All	0.37	1/9477 (0.0%)	0.57	1/12806 (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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	759	GLU	CG-CD	-5.10	1.44	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	759	GLU	OE1-CD-OE2	-5.52	116.67	123.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	759	GLU	Peptide
1	D	761	GLY	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	1174	0	1139	79	0
1	B	1173	0	1139	66	0
1	C	1178	0	1140	73	0
1	D	1188	0	1160	55	0
1	E	1170	0	1139	45	1
1	F	1156	0	1120	39	1
1	G	1127	0	1093	57	0
1	H	1133	0	1100	70	0
All	All	9299	0	9030	442	1

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 24.

The worst 5 of 442 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:684:HIS:HB3	1:A:686:ARG:HH12	1.26	1.00
1:G:796:ILE:HG13	1:G:815:ILE:HG12	1.47	0.96
1:A:684:HIS:HB3	1:A:686:ARG:NH1	1.88	0.87
1:A:789:LYS:HG3	1:G:748:LEU:HA	1.59	0.85
1:E:745:PHE:HB3	1:E:777:ALA:HB2	1.59	0.83

All (1) 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:E:719:GLU:OE2	1:F:686:ARG:NH1[1_664]	2.11	0.09

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	141/187 (75%)	133 (94%)	7 (5%)	1 (1%)	22	56
1	B	140/187 (75%)	138 (99%)	2 (1%)	0	100	100
1	C	141/187 (75%)	136 (96%)	5 (4%)	0	100	100
1	D	142/187 (76%)	136 (96%)	6 (4%)	0	100	100
1	E	140/187 (75%)	137 (98%)	3 (2%)	0	100	100
1	F	138/187 (74%)	134 (97%)	4 (3%)	0	100	100
1	G	135/187 (72%)	129 (96%)	5 (4%)	1 (1%)	22	56
1	H	136/187 (73%)	131 (96%)	5 (4%)	0	100	100
All	All	1113/1496 (74%)	1074 (96%)	37 (3%)	2 (0%)	47	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	762	ILE
1	G	762	ILE

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	124/157 (79%)	120 (97%)	4 (3%)	39	68
1	B	124/157 (79%)	121 (98%)	3 (2%)	49	74
1	C	125/157 (80%)	122 (98%)	3 (2%)	49	74

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	126/157 (80%)	123 (98%)	3 (2%)	49	74
1	E	124/157 (79%)	122 (98%)	2 (2%)	62	81
1	F	122/157 (78%)	119 (98%)	3 (2%)	47	73
1	G	119/157 (76%)	118 (99%)	1 (1%)	81	91
1	H	120/157 (76%)	119 (99%)	1 (1%)	81	91
All	All	984/1256 (78%)	964 (98%)	20 (2%)	55	77

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	789	LYS
1	F	808	TRP
1	H	743	TRP
1	G	743	TRP
1	B	848	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	699	GLN
1	F	754	GLN

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	145/187 (77%)	0.35	11 (7%)	13	17	28, 48, 99, 134	0
1	B	144/187 (77%)	0.24	5 (3%)	44	47	30, 45, 77, 98	0
1	C	145/187 (77%)	0.18	4 (2%)	53	57	34, 48, 66, 88	0
1	D	146/187 (78%)	0.40	9 (6%)	20	24	30, 52, 86, 106	0
1	E	144/187 (77%)	0.38	9 (6%)	20	23	44, 58, 82, 97	0
1	F	142/187 (75%)	0.54	12 (8%)	10	13	32, 58, 86, 115	0
1	G	139/187 (74%)	0.73	15 (10%)	5	7	39, 64, 91, 122	0
1	H	140/187 (74%)	0.37	6 (4%)	35	39	39, 55, 84, 103	0
All	All	1145/1496 (76%)	0.40	71 (6%)	20	24	28, 54, 86, 134	0

The worst 5 of 71 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	760	ASP	5.6
1	A	764	GLY	4.9
1	D	760	ASP	4.8
1	A	763	ALA	4.8
1	G	763	ALA	4.7

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.