wwPDB X-ray Structure Validation Summary Report (i)

May 25, 2020 – 05:14 am BST

PDB ID	:	6HPG
Title	:	Arabidopsis OM64 TPR domain
Authors	:	Schwenkert, S.
Deposited on	:	2018-09-20
Resolution	:	2.00 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 following versions of software and data (see references (1)) were used in the production of this report:

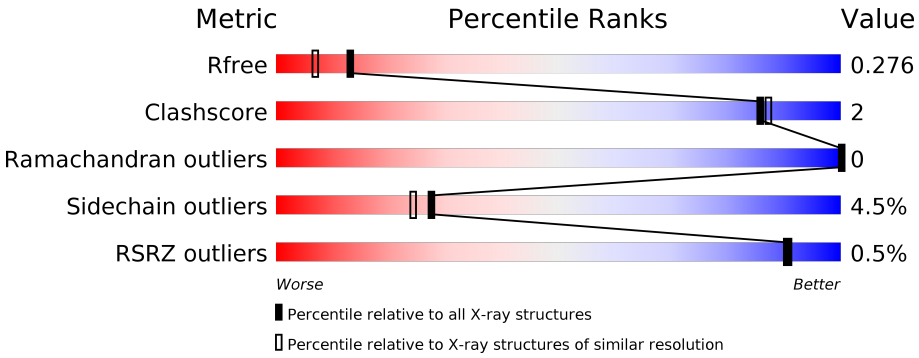
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 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.



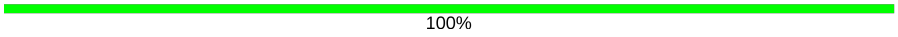
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	121	94% 6%
1	B	121	83% 11%
1	C	121	93%
1	D	121	90% 9%
1	E	121	88% 8%
1	F	121	91% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	a	8	
2	b	8	
2	c	8	
2	d	8	
2	e	8	
2	f	8	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6613 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 Outer envelope protein 64, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			965	604	179	175	7			
1	B	117	Total	C	N	O	S	0	0	0
			926	580	169	170	7			
1	C	117	Total	C	N	O	S	0	0	0
			926	580	169	170	7			
1	D	121	Total	C	N	O	S	0	1	0
			970	608	179	175	8			
1	E	117	Total	C	N	O	S	0	2	0
			937	587	171	172	7			
1	F	117	Total	C	N	O	S	0	0	0
			926	580	169	170	7			

- Molecule 2 is a protein called Heat shock protein 90-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	a	8	Total	C	N	O	S	0	0	0
			61	35	9	16	1			
2	b	8	Total	C	N	O	S	0	0	0
			61	35	9	16	1			
2	c	7	Total	C	N	O	S	0	0	0
			57	33	8	15	1			
2	d	8	Total	C	N	O	S	0	0	0
			61	35	9	16	1			
2	e	7	Total	C	N	O	S	0	0	0
			57	33	8	15	1			
2	f	7	Total	C	N	O	S	0	0	0
			57	33	8	15	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	107	Total O 107 107	0	0
3	B	87	Total O 87 87	0	0
3	C	100	Total O 100 100	0	0
3	D	92	Total O 92 92	0	0
3	E	78	Total O 78 78	0	0
3	F	79	Total O 79 79	0	0
3	a	12	Total O 12 12	0	0
3	b	12	Total O 12 12	0	0
3	c	12	Total O 12 12	0	0
3	d	12	Total O 12 12	0	0
3	e	10	Total O 10 10	0	0
3	f	8	Total O 8 8	0	0

3 Residue-property plots (i)

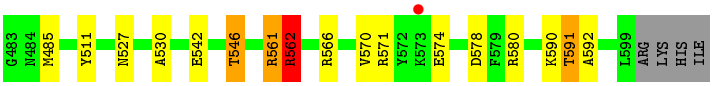
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Outer envelope protein 64, mitochondrial

Chain A:

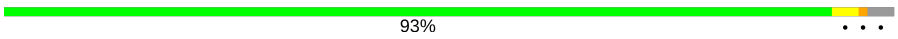
- Molecule 1: Outer envelope protein 64, mitochondrial

Chain B:



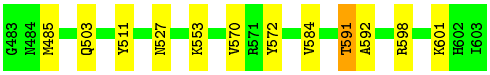
- Molecule 1: Outer envelope protein 64, mitochondrial

Chain C:



- Molecule 1: Outer envelope protein 64, mitochondrial

Chain D:



- Molecule 1: Outer envelope protein 64, mitochondrial

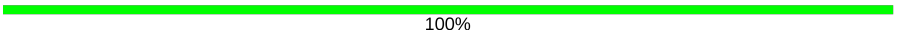
Chain E:

- Molecule 1: Outer envelope protein 64, mitochondrial

Chain F:

• Molecule 2: Heat shock protein 90-4

Chain a:



There are no outlier residues recorded for this chain.

• Molecule 2: Heat shock protein 90-4

Chain b:

• Molecule 2: Heat shock protein 90-4

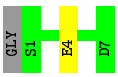
Chain c:

• Molecule 2: Heat shock protein 90-4

Chain d:

• Molecule 2: Heat shock protein 90-4

Chain e:



• Molecule 2: Heat shock protein 90-4

Chain f:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	29.39Å 61.13Å 106.56Å 87.57° 87.99° 78.26°	Depositor
Resolution (Å)	29.91 – 2.00 29.07 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.91-2.00) 92.7 (29.07-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.82 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.182 , 0.265 0.196 , 0.276	Depositor DCC
R_{free} test set	2395 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6613	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.3617e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.71	0/979	0.82	1/1308 (0.1%)
1	B	0.97	1/939 (0.1%)	0.85	2/1257 (0.2%)
1	C	1.01	1/939 (0.1%)	0.89	3/1257 (0.2%)
1	D	0.97	1/987 (0.1%)	0.77	2/1318 (0.2%)
1	E	0.65	0/956	0.77	0/1280
1	F	0.64	0/939	0.75	1/1257 (0.1%)
2	a	0.74	0/60	0.72	0/76
2	b	0.65	0/60	0.75	0/76
2	c	0.60	0/56	0.92	0/71
2	d	0.74	0/60	0.87	0/76
2	e	0.74	0/56	0.85	0/71
2	f	0.61	0/56	0.81	0/71
All	All	0.83	3/6087 (0.0%)	0.81	9/8118 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	591	THR	C-N	23.18	1.87	1.34
1	D	591	THR	C-N	21.41	1.83	1.34
1	B	591	THR	C-N	19.69	1.79	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	591	THR	O-C-N	-17.16	95.25	122.70
1	B	561	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	F	528	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	561	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	578	ASP	CB-CG-OD2	-5.36	113.47	118.30

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	965	0	978	3	0
1	B	926	0	933	10	0
1	C	926	0	933	2	0
1	D	970	0	986	6	0
1	E	937	0	948	5	0
1	F	926	0	934	1	0
2	a	61	0	57	0	0
2	b	61	0	57	0	0
2	c	57	0	54	0	0
2	d	61	0	57	0	0
2	e	57	0	54	0	0
2	f	57	0	54	0	0
3	A	107	0	0	2	0
3	B	87	0	0	0	1
3	C	100	0	0	0	0
3	D	92	0	0	0	0
3	E	78	0	0	1	0
3	F	79	0	0	0	1
3	a	12	0	0	0	0
3	b	12	0	0	0	0
3	c	12	0	0	0	0
3	d	12	0	0	0	0
3	e	10	0	0	0	0
3	f	8	0	0	0	0
All	All	6613	0	6045	25	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 2.

The worst 5 of 25 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:B:591:THR:C	1:B:592:ALA:N	1.79	1.36
1:D:591:THR:C	1:D:592:ALA:N	1.83	1.29
1:C:591:THR:C	1:C:592:ALA:N	1.87	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:THR:HG22	1:B:562:ARG:HE	1.55	0.70
1:D:591:THR:C	1:D:592:ALA:CA	2.67	0.63

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)
3:B:702:HOH:O	3:F:724:HOH:O[1_645]	1.79	0.41

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	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
1	B	115/121 (95%)	110 (96%)	5 (4%)	0	100	100
1	C	115/121 (95%)	113 (98%)	2 (2%)	0	100	100
1	D	120/121 (99%)	117 (98%)	3 (2%)	0	100	100
1	E	117/121 (97%)	114 (97%)	3 (3%)	0	100	100
1	F	115/121 (95%)	112 (97%)	3 (3%)	0	100	100
2	a	6/8 (75%)	5 (83%)	1 (17%)	0	100	100
2	b	6/8 (75%)	6 (100%)	0	0	100	100
2	c	5/8 (62%)	5 (100%)	0	0	100	100
2	d	6/8 (75%)	6 (100%)	0	0	100	100
2	e	5/8 (62%)	5 (100%)	0	0	100	100
2	f	5/8 (62%)	5 (100%)	0	0	100	100
All	All	734/774 (95%)	714 (97%)	20 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	96/96 (100%)	93 (97%)	3 (3%)	40	40
1	B	92/96 (96%)	86 (94%)	6 (6%)	17	12
1	C	92/96 (96%)	90 (98%)	2 (2%)	52	55
1	D	97/96 (101%)	92 (95%)	5 (5%)	23	19
1	E	94/96 (98%)	90 (96%)	4 (4%)	29	26
1	F	92/96 (96%)	88 (96%)	4 (4%)	29	26
2	a	7/7 (100%)	7 (100%)	0	100	100
2	b	7/7 (100%)	6 (86%)	1 (14%)	3	1
2	c	7/7 (100%)	6 (86%)	1 (14%)	3	1
2	d	7/7 (100%)	6 (86%)	1 (14%)	3	1
2	e	7/7 (100%)	6 (86%)	1 (14%)	3	1
2	f	7/7 (100%)	6 (86%)	1 (14%)	3	1
All	All	605/618 (98%)	576 (95%)	29 (5%)	27	22

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	503	GLN
1	E	503[A]	GLN
2	d	4	GLU
1	D	553	LYS
1	E	503[B]	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	543	GLN
1	F	543	GLN
1	D	496	ASN
1	B	505	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	503	GLN

5.3.3 RNA

There are no RNA molecules 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	591:THR	C	592:ALA	N	1.87
1	D	591:THR	C	592:ALA	N	1.83
1	B	591:THR	C	592:ALA	N	1.79

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	121/121 (100%)	-0.48	1 (0%) 86 85	14, 24, 44, 68	0
1	B	117/121 (96%)	-0.37	1 (0%) 84 83	20, 27, 48, 55	0
1	C	117/121 (96%)	-0.46	0 100 100	17, 25, 48, 65	0
1	D	121/121 (100%)	-0.43	0 100 100	15, 26, 47, 65	0
1	E	117/121 (96%)	-0.42	2 (1%) 70 68	17, 27, 58, 89	0
1	F	117/121 (96%)	-0.39	0 100 100	17, 30, 53, 61	0
2	a	8/8 (100%)	-0.64	0 100 100	22, 32, 37, 49	0
2	b	8/8 (100%)	-0.42	0 100 100	26, 35, 47, 59	0
2	c	7/8 (87%)	-0.16	0 100 100	28, 40, 53, 54	0
2	d	8/8 (100%)	-0.31	0 100 100	28, 40, 52, 54	0
2	e	7/8 (87%)	-0.37	0 100 100	31, 34, 42, 50	0
2	f	7/8 (87%)	-0.18	0 100 100	30, 44, 55, 60	0
All	All	755/774 (97%)	-0.42	4 (0%) 91 90	14, 27, 53, 89	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	599	LEU	3.8
1	A	570	VAL	3.0
1	B	573	LYS	2.7
1	E	597	LYS	2.6

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 (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.