



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 16, 2024 – 08:54 PM EDT

PDB ID : 5OJR
Title : YCF48 bound to D1 peptide
Authors : Michoux, F.; Nixon, P.J.; Murray, J.W.; Bialek, W.; Thieulin-Pardo, G.
Deposited on : 2017-07-23
Resolution : 1.96 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 ⓘ 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 ⓘ](#)) 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

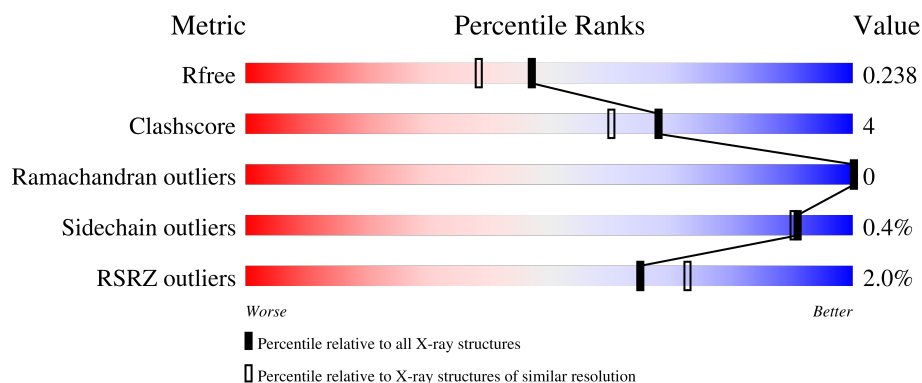
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 $\leq 5\%$. 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	326	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>6%</div> </div> </div>
1	B	326	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>5%</div> </div> </div>
1	C	326	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>6%</div> <div>8%</div> </div> </div>
1	D	326	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>6%</div> <div>7%</div> </div> </div>
2	E	18	<div> <div></div> <div> <div>89%</div> <div>11%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	F	18	<div> <div>6%</div> <div>83%</div> <div>11%</div> <div>6%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10323 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 Ycf48-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2407	1528	421	450	8			
1	B	310	Total	C	N	O	S	0	0	0
			2427	1539	429	451	8			
1	C	301	Total	C	N	O	S	0	0	0
			2350	1492	408	442	8			
1	D	303	Total	C	N	O	S	0	0	0
			2367	1502	412	445	8			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	MET	-	initiating methionine	UNP Q8DI95
A	23	ARG	-	expression tag	UNP Q8DI95
A	24	GLY	-	expression tag	UNP Q8DI95
A	25	SER	-	expression tag	UNP Q8DI95
A	26	HIS	-	expression tag	UNP Q8DI95
A	27	HIS	-	expression tag	UNP Q8DI95
A	28	HIS	-	expression tag	UNP Q8DI95
A	29	HIS	-	expression tag	UNP Q8DI95
A	30	HIS	-	expression tag	UNP Q8DI95
A	31	HIS	-	expression tag	UNP Q8DI95
A	32	GLY	-	expression tag	UNP Q8DI95
A	33	LEU	-	expression tag	UNP Q8DI95
A	34	VAL	-	expression tag	UNP Q8DI95
A	35	PRO	-	expression tag	UNP Q8DI95
A	36	ARG	-	expression tag	UNP Q8DI95
A	37	GLY	-	expression tag	UNP Q8DI95
A	38	SER	-	expression tag	UNP Q8DI95
B	22	MET	-	initiating methionine	UNP Q8DI95
B	23	ARG	-	expression tag	UNP Q8DI95
B	24	GLY	-	expression tag	UNP Q8DI95
B	25	SER	-	expression tag	UNP Q8DI95

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	HIS	-	expression tag	UNP Q8DI95
B	27	HIS	-	expression tag	UNP Q8DI95
B	28	HIS	-	expression tag	UNP Q8DI95
B	29	HIS	-	expression tag	UNP Q8DI95
B	30	HIS	-	expression tag	UNP Q8DI95
B	31	HIS	-	expression tag	UNP Q8DI95
B	32	GLY	-	expression tag	UNP Q8DI95
B	33	LEU	-	expression tag	UNP Q8DI95
B	34	VAL	-	expression tag	UNP Q8DI95
B	35	PRO	-	expression tag	UNP Q8DI95
B	36	ARG	-	expression tag	UNP Q8DI95
B	37	GLY	-	expression tag	UNP Q8DI95
B	38	SER	-	expression tag	UNP Q8DI95
C	22	MET	-	initiating methionine	UNP Q8DI95
C	23	ARG	-	expression tag	UNP Q8DI95
C	24	GLY	-	expression tag	UNP Q8DI95
C	25	SER	-	expression tag	UNP Q8DI95
C	26	HIS	-	expression tag	UNP Q8DI95
C	27	HIS	-	expression tag	UNP Q8DI95
C	28	HIS	-	expression tag	UNP Q8DI95
C	29	HIS	-	expression tag	UNP Q8DI95
C	30	HIS	-	expression tag	UNP Q8DI95
C	31	HIS	-	expression tag	UNP Q8DI95
C	32	GLY	-	expression tag	UNP Q8DI95
C	33	LEU	-	expression tag	UNP Q8DI95
C	34	VAL	-	expression tag	UNP Q8DI95
C	35	PRO	-	expression tag	UNP Q8DI95
C	36	ARG	-	expression tag	UNP Q8DI95
C	37	GLY	-	expression tag	UNP Q8DI95
C	38	SER	-	expression tag	UNP Q8DI95
D	22	MET	-	initiating methionine	UNP Q8DI95
D	23	ARG	-	expression tag	UNP Q8DI95
D	24	GLY	-	expression tag	UNP Q8DI95
D	25	SER	-	expression tag	UNP Q8DI95
D	26	HIS	-	expression tag	UNP Q8DI95
D	27	HIS	-	expression tag	UNP Q8DI95
D	28	HIS	-	expression tag	UNP Q8DI95
D	29	HIS	-	expression tag	UNP Q8DI95
D	30	HIS	-	expression tag	UNP Q8DI95
D	31	HIS	-	expression tag	UNP Q8DI95
D	32	GLY	-	expression tag	UNP Q8DI95
D	33	LEU	-	expression tag	UNP Q8DI95

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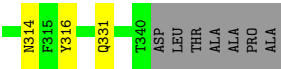
Chain	Residue	Modelled	Actual	Comment	Reference
D	34	VAL	-	expression tag	UNP Q8DI95
D	35	PRO	-	expression tag	UNP Q8DI95
D	36	ARG	-	expression tag	UNP Q8DI95
D	37	GLY	-	expression tag	UNP Q8DI95
D	38	SER	-	expression tag	UNP Q8DI95

- Molecule 2 is a protein called Photosystem II protein D1 3.

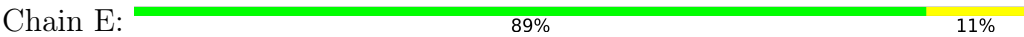
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	18	Total	C	N	O	0	0	0
			129	80	22	27			
2	F	17	Total	C	N	O	0	0	0
			123	77	21	25			

- Molecule 3 is water.

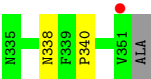
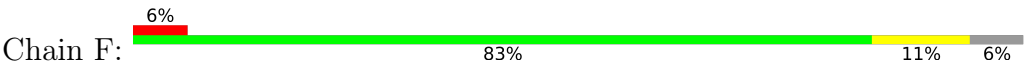
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	115	Total	O	0	0
			115	115		
3	B	168	Total	O	0	0
			168	168		
3	C	98	Total	O	0	0
			98	98		
3	D	124	Total	O	0	0
			124	124		
3	E	8	Total	O	0	0
			8	8		
3	F	7	Total	O	0	0
			7	7		



● Molecule 2: Photosystem II protein D1 3



● Molecule 2: Photosystem II protein D1 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.32Å 60.46Å 103.46Å 90.00° 96.78° 90.00°	Depositor
Resolution (Å)	74.94 – 1.96 74.95 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.3 (74.94-1.96) 99.3 (74.95-1.96)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.193 , 0.238 0.195 , 0.238	Depositor DCC
R_{free} test set	4130 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 51.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10323	wwPDB-VP
Average B, all atoms (Å ²)	29.0	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 59.39 % 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 1.7775e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	0.48	0/2475	0.68	1/3372 (0.0%)
1	B	0.52	0/2495	0.68	0/3397
1	C	0.43	0/2416	0.65	1/3293 (0.0%)
1	D	0.50	0/2434	0.70	2/3318 (0.1%)
2	E	0.39	0/132	0.52	0/180
2	F	0.39	0/126	0.51	0/173
All	All	0.48	0/10078	0.67	4/13733 (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	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	GLU	N-CA-CB	5.97	121.36	110.60
1	D	39	ILE	CG1-CB-CG2	5.77	124.09	111.40
1	D	169	ASP	CB-CG-OD1	5.23	123.01	118.30
1	C	175	GLN	CB-CA-C	-5.12	100.16	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	256	GLU	Sidechain

5.2 Too-close contacts ⓘ

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	2407	0	2318	27	1
1	B	2427	0	2345	20	1
1	C	2350	0	2255	10	1
1	D	2367	0	2275	16	1
2	E	129	0	117	2	0
2	F	123	0	112	1	0
3	A	115	0	0	1	0
3	B	168	0	0	0	0
3	C	98	0	0	1	0
3	D	124	0	0	1	0
3	E	8	0	0	0	0
3	F	7	0	0	0	0
All	All	10323	0	9422	73	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 4.

The worst 5 of 73 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:D:314:ASN:H	1:D:331:GLN:HE21	1.18	0.90
1:D:314:ASN:H	1:D:331:GLN:NE2	1.78	0.82
1:D:297:ASP:O	1:D:300:GLN:HG3	1.87	0.75
1:B:52:LEU:HD22	1:B:79:MET:HE1	1.71	0.72
1:A:316:TYR:HE2	1:A:331:GLN:HG2	1.55	0.71

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:A:224:SER:OG	1:D:307:ASP:OD2[2_755]	2.03	0.17
1:B:224:SER:OG	1:C:307:ASP:OD2[2_856]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	304/326 (93%)	299 (98%)	5 (2%)	0	100	100
1	B	306/326 (94%)	300 (98%)	6 (2%)	0	100	100
1	C	297/326 (91%)	292 (98%)	5 (2%)	0	100	100
1	D	301/326 (92%)	298 (99%)	3 (1%)	0	100	100
2	E	16/18 (89%)	15 (94%)	1 (6%)	0	100	100
2	F	15/18 (83%)	15 (100%)	0	0	100	100
All	All	1239/1340 (92%)	1219 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	257/272 (94%)	256 (100%)	1 (0%)	91	90
1	B	259/272 (95%)	259 (100%)	0	100	100
1	C	251/272 (92%)	251 (100%)	0	100	100
1	D	253/272 (93%)	251 (99%)	2 (1%)	81	80
2	E	13/13 (100%)	13 (100%)	0	100	100
2	F	13/13 (100%)	12 (92%)	1 (8%)	13	4
All	All	1046/1114 (94%)	1042 (100%)	4 (0%)	91	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	ASP
1	D	229	ASN
1	D	243	ASN
2	F	338	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	229	ASN
1	D	243	ASN
1	D	331	GLN
1	B	213	GLN
1	C	75	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	308/326 (94%)	-0.04	6 (1%) 66 74	17, 27, 52, 94	0
1	B	310/326 (95%)	-0.17	5 (1%) 72 79	12, 22, 46, 81	0
1	C	301/326 (92%)	0.00	7 (2%) 60 69	17, 30, 55, 79	0
1	D	303/326 (92%)	-0.11	6 (1%) 65 73	14, 25, 49, 94	0
2	E	18/18 (100%)	0.03	0 100 100	24, 32, 46, 50	0
2	F	17/18 (94%)	0.27	1 (5%) 22 30	17, 24, 45, 68	0
All	All	1257/1340 (93%)	-0.07	25 (1%) 65 73	12, 26, 52, 94	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	269	SER	5.5
1	D	268	ASN	4.9
1	C	44	TYR	4.9
2	F	351	VAL	4.5
1	C	223	THR	4.2

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.