

wwPDB X-ray Structure Validation Summary Report (i)

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PDB ID	:	2GCJ
Title	:	Crystal Structure of the Pob3 middle domain
Authors	:	VanDemark, A.P.
Deposited on	:	2006-03-14
Resolution	:	2.55 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	:	2.23.2
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)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.55 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	$\begin{array}{c} {\rm Whole \ archive} \\ {\rm (\#Entries)} \end{array}$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(Å)}) \end{array}$
R _{free}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 c	hain	
1	А	261	^{2%} 58%	26%	•• 12%
1	В	261	% 63%	20%	5%• 12%
1	С	261	57%	25%	6% 11%
1	D	261	% 56%	26%	5%• 12%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7649 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 Hypothetical 63.0 kDa protein in DAK1-ORC1 intergenic region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1 1	220	Total	С	Ν	0	S	0	0	0
1	A	229	1888	1210	321	354	3	0		
1	Р	220	Total	С	Ν	0	S	3	0	0
1	ГБ	230	1895	1215	322	355	3			
1	C	0.01	Total	С	Ν	0	S	F	0	0
	231	1904	1220	323	358	3	5	0		
1 D	229	Total	С	Ν	0	S	0	0	0	
		1882	1207	318	354	3			U	

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	218	GLY	-	cloning artifact	UNP Q04636
А	219	HIS	-	cloning artifact	UNP Q04636
А	308	LYS	GLN	engineered mutation	UNP Q04636
В	218	GLY	-	cloning artifact	UNP Q04636
В	219	HIS	-	cloning artifact	UNP Q04636
В	308	LYS	GLN	engineered mutation	UNP Q04636
С	218	GLY	-	cloning artifact	UNP Q04636
С	219	HIS	-	cloning artifact	UNP Q04636
С	308	LYS	GLN	engineered mutation	UNP Q04636
D	218	GLY	-	cloning artifact	UNP Q04636
D	219	HIS	-	cloning artifact	UNP Q04636
D	308	LYS	GLN	engineered mutation	UNP Q04636

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	21	Total O 21 21	0	0
2	В	25	TotalO2525	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	18	Total O 18 18	0	0
2	D	16	Total O 16 16	0	0



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: Hypothetical 63.0 kDa protein in DAK1-ORC1 intergenic region



P413 F414 F433 F433 F433 F434 F445 F446 F446 F446 F446 F446 F446 F446 F446 F446 F447 F446 F447 F447 F446 F447 F447 F447 F447 F447 F447 F447 F447 F447 F457 F458

• Molecule 1: Hypothetical 63.0 kDa protein in DAK1-ORC1 intergenic region





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	57.87Å 157.53Å 57.79Å	Deperitor
a, b, c, α , β , γ	90.00° 89.77° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	78.81 - 2.55	Depositor
Resolution (A)	$32.30 \ - \ 2.49$	EDS
% Data completeness	91.7 (78.81-2.55)	Depositor
(in resolution range)	91.1 (32.30-2.49)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.08 (at 2.51 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
B B.	0.215 , 0.303	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.217 , 0.299	DCC
R_{free} test set	1638 reflections (4.99%)	wwPDB-VP
Wilson B-factor $(Å^2)$	45.9	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 6.2	EDS
L-test for twinning ²	$< L > = 0.52, < L^2 > = 0.35$	Xtriage
	0.000 for l,k,-h	
Estimated twinning fraction	0.460 for -h,-k,l	Xtriage
	0.000 for -l,-k,-h	
F_o, F_c correlation	0.95	EDS
Total number of atoms	7649	wwPDB-VP
Average B, all atoms $(Å^2)$	38.0	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 38.28 % 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 3.7782e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

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		
WIOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.57	0/1926	0.70	1/2599~(0.0%)	
1	В	0.63	0/1933	0.74	0/2609	
1	С	0.62	0/1942	0.75	0/2621	
1	D	0.57	0/1920	0.70	0/2592	
All	All	0.60	0/7721	0.72	1/10421~(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	А	0	1
1	В	0	3
1	С	0	1
1	D	0	4
All	All	0	9

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	А	254	ARG	NE-CZ-NH1	5.29	122.94	120.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	407	LYS	Peptide
1	В	339	GLU	Peptide
1	В	382	CYS	Peptide
1	В	405	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	\mathbf{C}	407	LYS	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	А	1888	0	1890	55	0
1	В	1895	0	1899	45	0
1	С	1904	0	1905	78	0
1	D	1882	0	1879	67	0
2	А	21	0	0	0	0
2	В	25	0	0	3	0
2	С	18	0	0	0	0
2	D	16	0	0	0	0
All	All	7649	0	7573	238	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 16.

The worst 5 of 238 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:C:294:ILE:HD11	1:C:295:HIS:CE1	1.76	1.20
1:B:339:GLU:OE2	1:B:339:GLU:HA	1.49	1.11
1:D:252:THR:HG22	1:D:253:PRO:HD3	1.38	1.05
1:D:406:THR:O	1:D:407:LYS:HG3	1.55	1.05
1:C:371:VAL:HB	1:C:372:PRO:HD2	1.39	1.04

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.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	А	225/261~(86%)	197~(88%)	26 (12%)	2(1%)	17	24
1	В	226/261~(87%)	203~(90%)	21 (9%)	2(1%)	17	24
1	С	227/261~(87%)	212~(93%)	13~(6%)	2(1%)	17	24
1	D	225/261~(86%)	210~(93%)	11 (5%)	4 (2%)	8	10
All	All	903/1044 (86%)	822 (91%)	71 (8%)	10 (1%)	14	19

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	В	406	THR
1	D	322	LYS
1	D	406	THR
1	А	292	ASP
1	С	366	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	211/237~(89%)	192~(91%)	19 (9%)	9	11
1	В	212/237~(90%)	182~(86%)	30 (14%)	3	3
1	С	213/237~(90%)	190 (89%)	23~(11%)	6	6
1	D	210/237~(89%)	186~(89%)	24 (11%)	5	5
All	All	846/948~(89%)	750(89%)	96 (11%)	6	5

 $5~{\rm of}~96$ residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	С	326	THR
1	С	474	ASN

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Mol	Chain	Res	Type
1	С	338	GLU
1	С	378	LYS
1	D	266	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	348	GLN
1	D	452	ASN
1	С	319	GLN
1	С	321	GLN
1	С	340	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, 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	А	229/261~(87%)	0.12	6 (2%) 56 62	15, 41, 75, 105	2 (0%)
1	В	230/261~(88%)	-0.08	2 (0%) 84 88	9, 31, 65, 94	1 (0%)
1	С	231/261~(88%)	-0.13	1 (0%) 92 96	7, 30, 65, 100	2 (0%)
1	D	229/261~(87%)	0.02	3 (1%) 77 82	15, 41, 77, 113	0
All	All	919/1044~(88%)	-0.02	12 (1%) 77 82	7, 36, 73, 113	5 (0%)

The worst 5 of 12 RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	В	237	VAL	3.8
1	А	466	LYS	3.0
1	А	422	ILE	3.0
1	А	340	ASN	2.8
1	D	310	GLN	2.5

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.

