

# Full wwPDB X-ray Structure Validation Report (i)

Nov 20, 2023 – 04:17 PM JST

PDB ID : 7CYZ

Title: The structure of human ORP3 OSBP-related domain

Authors : Dong, X. Deposited on : 2020-09-05

Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$ 

CCP4 : 7.0.044 (Gargrove)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

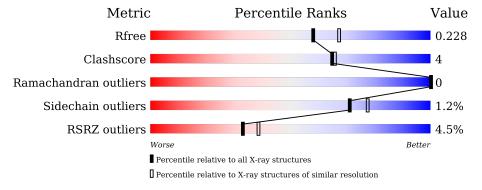
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.10 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\#  ext{Entries},  ext{ resolution range}( ext{Å}))$
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	377	85%	8% • 6%
1	В	377	90%	10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:



Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CAF	В	515	-	-	-	X



# 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6588 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 Oxysterol-binding protein-related protein 3.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace		
1	A	355	Total 2950	As 3	C 1872	N 520	O 541	S 14	0	1	0
1	В	377	Total 3133	As 3	C 1987	N 554	O 575	S 14	0	2	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	579	ILE	LEU	engineered mutation	· •
A	615	ARG	CYS	engineered mutation	UNP Q9H4L5
В	579	ILE	LEU	engineered mutation	UNP Q9H4L5
В	615	ARG	CYS	engineered mutation	UNP Q9H4L5

• Molecule 2 is water.

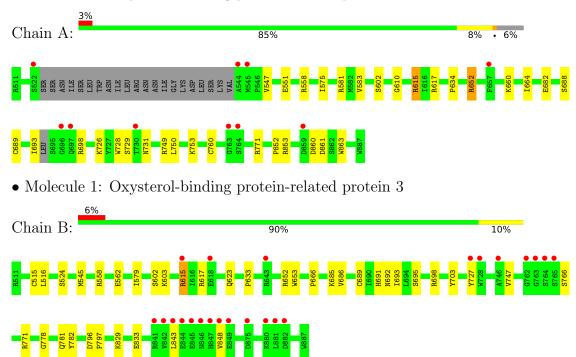
ľ	Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
	2	A	288	Total O 288 288	0	0
	2	В	217	Total O 217 217	0	0



# 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: Oxysterol-binding protein-related protein 3





# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants	95.34Å 95.34Å 185.25Å	Domositon
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	41.28 - 2.10	Depositor
Resolution (A)	41.28 - 2.10	EDS
% Data completeness	99.8 (41.28-2.10)	Depositor
(in resolution range)	99.8 (41.28-2.10)	EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	3.10 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
D.D.	0.173 , 0.219	Depositor
$R, R_{free}$	0.189 , $0.228$	DCC
$R_{free}$ test set	2920 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.3	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.34, 56.0	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.50, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

### 5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CAF

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		
IVIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	A	0.49	0/3003	0.56	0/4058	
1	В	0.43	0/3190	0.53	0/4314	
All	All	0.46	0/6193	0.54	0/8372	

There are no bond length outliers.

There are no bond angle outliers.

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	2950	0	2803	23	0
1	В	3133	0	2998	29	0
2	A	288	0	0	3	0
2	В	217	0	0	1	0
All	All	6588	0	5801	49	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 4.

All (49) 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:615:ARG:HH21	1:B:615:ARG:HG2	1.37	0.90
1:B:515:CAF:HB3	1:B:782:TYR:CE2	2.09	0.86
1:A:615:ARG:HD3	1:A:617:ARG:HD3	1.61	0.80
1:B:615:ARG:HG2	1:B:615:ARG:NH2	1.98	0.76
1:B:562:GLU:OE2	1:B:685:LYS:NZ	2.29	0.65
1:B:615:ARG:HD3	1:B:617:ARG:HG2	1.80	0.64
1:A:771:ARG:NH1	1:B:727:TYR:O	2.34	0.61
1:A:693:ILE:O	1:A:698:ARG:NH1	2.35	0.59
1:A:749:ARG:NH2	2:A:903:HOH:O	2.35	0.59
1:A:615:ARG:O	1:A:615:ARG:HG3	2.03	0.59
1:A:610:GLY:O	1:A:853:ARG:NH1	2.36	0.58
1:B:515:CAF:HB3	1:B:782:TYR:HE2	1.63	0.57
1:A:634:PRO:O	1:A:652:ARG:HG2	2.05	0.56
1:A:726:LYS:HE3	1:A:728:TRP:CH2	2.39	0.56
1:B:615:ARG:CD	1:B:617:ARG:HG2	2.36	0.56
1:B:615:ARG:NE	1:B:617:ARG:HD3	2.21	0.55
1:B:633:PRO:HB2	1:B:652:ARG:HD2	1.89	0.55
1:A:615:ARG:HH11	1:A:617:ARG:HH11	1.56	0.53
1:B:558:ARG:NH2	1:B:602:SER:OG	2.41	0.53
1:B:692:ASN:HB3	1:B:695:SER:HB3	1.91	0.53
1:B:829:LYS:O	1:B:833:GLU:HG2	2.10	0.51
1:B:689:CAF:O1	1:B:691:HIS:CE1	2.64	0.51
1:A:749:ARG:HH21	1:B:766:SER:HB3	1.77	0.49
1:A:575:ILE:O	1:A:581:ARG:HD3	2.12	0.49
1:B:686:VAL:HB	1:B:703:TYR:O	2.13	0.49
1:B:515:CAF:SG	1:B:516:LEU:N	2.85	0.48
1:B:829:LYS:NZ	2:B:909:HOH:O	2.45	0.48
1:B:615:ARG:HH21	1:B:615:ARG:CG	2.14	0.47
1:A:729:SER:HB3	2:A:1029:HOH:O	2.14	0.47
1:A:852:PRO:HG2	1:A:863:TRP:CZ3	2.50	0.46
1:B:689:CAF:O1	1:B:691:HIS:HE1	1.98	0.46
1:B:545:MET:SD	1:B:603:LYS:NZ	2.82	0.45
1:A:583:VAL:HG13	1:A:750:LEU:HD21	1.99	0.44
1:A:615:ARG:HD3	1:A:617:ARG:CD	2.38	0.43
1:A:551:GLU:HB3	1:A:602:SER:HB2	2.01	0.43
1:B:843:LEU:HD22	1:B:848:VAL:HB	2.01	0.42
1:B:653:TRP:CZ3	1:B:666:PRO:HB3	2.54	0.42
1:A:615:ARG:HA	1:A:615:ARG:HE	1.85	0.42
1:A:693:ILE:HD12	1:A:693:ILE:HA	1.93	0.41
1:A:660:LYS:HG2	2:A:1060:HOH:O	2.20	0.41
1:A:860:ASP:O	1:A:861:ASP:HB2	2.21	0.41
1:B:693:ILE:O	1:B:698:ARG:NH1	2.53	0.41

Continued on next page...



$\alpha \cdots$	c		
Continued	trom	nrevious	naae

Atom-1	Atom-2	Interatomic	Clash
		distance (Å)	overlap (Å)
1:A:664:ILE:HB	1:A:688:SER:HB2	2.01	0.41
1:B:778:GLY:O	1:B:781:GLN:HG2	2.21	0.41
1:B:615:ARG:NH2	1:B:615:ARG:CG	2.73	0.40
1:B:796:ASP:HA	1:B:797:PRO:HD3	1.82	0.40
1:A:558[B]:ARG:HA	1:A:558[B]:ARG:HD2	1.94	0.40
1:A:753:LYS:HE2	1:B:771:ARG:NH1	2.36	0.40
1:B:579:ILE:HD13	1:B:747:VAL:HG11	2.04	0.40

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.

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	Perce	ntiles
1	A	347/377 (92%)	337 (97%)	10 (3%)	0	100	100
1	В	374/377 (99%)	360 (96%)	14 (4%)	0	100	100
All	All	721/754 (96%)	697 (97%)	24 (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	Rotameric Outliers	
1	A	316/336 (94%)	311 (98%)	5 (2%)	62 69

 $\overline{C}$  ontinued on next page...



Continued from previous page...

Mol	Chain	Analysed	Rotameric	meric Outliers		Percentiles		
1	В	338/336 (101%)	335 (99%)	3 (1%)	78	84		
All	All	654/672 (97%)	646 (99%)	8 (1%)	71	77		

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	VAL
1	A	615	ARG
1	A	652	ARG
1	A	682	GLU
1	A	731	ASN
1	В	524	SER
1	В	615	ARG
1	В	623	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	$\operatorname{Res}$	Type
1	A	655	ASN
1	A	731	ASN
1	A	850	HIS
1	В	691	HIS

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

#### 5.4 Non-standard residues in protein, DNA, RNA chains (i)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Iol Type Chain Res		Link	В	Bond lengths			Bond angles		
MIOI	туре	Chain	nes	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CAF	A	760	1	3,9,10	0.74	0	1,12,14	3.35	1 (100%)
1	CAF	A	515	1	3,9,10	0.83	0	1,12,14	1.68	0
1	CAF	В	689	1	3,9,10	0.94	0	1,12,14	1.17	0
1	CAF	В	760	1	3,9,10	0.93	0	1,12,14	1.45	0
1	CAF	В	515	1	3,9,10	0.92	0	1,12,14	1.17	0
1	CAF	A	689	1	3,9,10	0.93	0	1,12,14	2.28	1 (100%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAF	A	760	1	-	0/0/8/10	-
1	CAF	A	515	1	-	0/0/8/10	-
1	CAF	В	689	1	-	0/0/8/10	-
1	CAF	В	760	1	-	0/0/8/10	-
1	CAF	В	515	1	-	0/0/8/10	-
1	CAF	A	689	1	-	0/0/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
1	A	760	CAF	CA-CB-SG	-3.35	105.79	112.76
1	A	689	CAF	CA-CB-SG	-2.28	108.01	112.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	В	689	CAF	2	0
1	В	515	CAF	3	0

#### 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 $>$	#RSR	RZ>2	$\mathbf{OWAB}(\mathbf{\mathring{A}}^2)$	Q < 0.9
1	A	352/377~(93%)	-0.18	10 (2%)	53 59	14, 29, 62, 108	0
1	В	374/377 (99%)	-0.05	23 (6%)	21 26	20, 39, 76, 119	0
All	All	726/754 (96%)	-0.12	33 (4%)	33 38	14, 34, 74, 119	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	763	GLY	4.5
1	В	847	HIS	4.3
1	В	762	GLY	4.2
1	В	763	GLY	4.2
1	В	848	VAL	4.1
1	В	842	VAL	3.7
1	В	728	TRP	3.5
1	В	764	SER	3.4
1	В	846	ASN	3.3
1	A	697	GLN	3.3
1	В	841	ARG	3.3
1	A	859	ASP	3.1
1	A	657	PHE	3.1
1	В	618	GLU	3.1
1	В	845	GLU	3.0
1	В	875	ASP	2.9
1	В	849	GLU	2.9
1	В	843	LEU	2.9
1	В	765	SER	2.9
1	В	880	LYS	2.8
1	A	696	GLY	2.8
1	A	764	SER	2.8
1	В	727	TYR	2.7
1	A	545	MET	2.5

Continued on next page...



Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	В	615	ARG	2.4
1	В	882	ASP	2.4
1	В	881	LEU	2.4
1	A	544	ALA	2.4
1	В	844	GLU	2.3
1	A	730	THR	2.2
1	В	746	ALA	2.2
1	A	522	SER	2.0
1	В	643	ARG	2.0

#### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median,  $95^{th}$  percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
1	CAF	В	515	10/11	0.53	0.59	20,20,20,20	0
1	CAF	A	689	10/11	0.94	0.12	24,27,132,135	0
1	CAF	A	515	10/11	0.94	0.12	22,30,125,151	0
1	CAF	A	760	10/11	0.95	0.13	21,40,72,72	0
1	CAF	В	760	10/11	0.97	0.11	21,29,67,161	0
1	CAF	В	689	10/11	0.98	0.10	22,30,41,177	0

### 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.

