

Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 07:11 AM EDT

PDB ID : 6WMG

Title : Human Sun2 (500-717) Authors : Cruz, V.E.; Schwartz, T.U.

Deposited on : 2020-04-21

Resolution : 1.90 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 Xtriage (Phenix) : 1.13

EDS : 2.35.1

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

Refmac : 5.8.0158

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

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

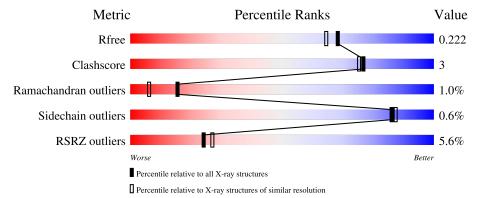
Validation Pipeline (wwPDB-VP) : 2.35.1

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 1.90 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 $(\# \mathrm{Entries})$	Similar resolution $(\# \text{Entries, resolution range}(\text{\AA}))$
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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		
			5%		
1	A	224	79%	8%	13%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1671 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 SUN domain-containing protein 2.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Δ	195	Total	С	N	О	S	0	9	0
1	11	150	1540	983	265	288	4		2	U

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	494	GLY	-	expression tag	UNP Q9UH99
A	495	PRO	-	expression tag	UNP Q9UH99
A	496	GLY	-	expression tag	UNP Q9UH99
A	497	GLY	-	expression tag	UNP Q9UH99
A	498	SER	-	expression tag	UNP Q9UH99
A	499	GLY	-	expression tag	UNP Q9UH99

• Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0

• Molecule 3 is water.

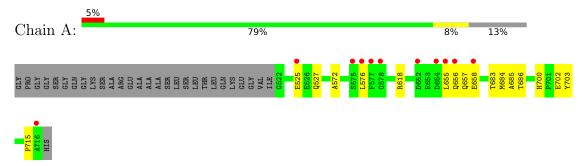
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	130	Total O 130 130	0	0



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: SUN domain-containing protein 2





4 Data and refinement statistics (i)

$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Property	Value	Source
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Space group	H 3 2	Depositor
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Cell constants	79.19Å 79.19Å 199.47Å	Donositon
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		56.51 - 1.90	Depositor
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Resolution (A)		EDS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	% Data completeness	98.2 (56.51-1.90)	Depositor
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	(in resolution range)	98.2 (56.51-1.90)	EDS
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	R_{merge}	(Not available)	Depositor
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	R_{sym}	(Not available)	Depositor
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$< I/\sigma(I) > 1$	1.16 (at 1.90Å)	Xtriage
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Refinement program	PHENIX 1.17_3644	Depositor
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	D D	0.175 , 0.223	Depositor
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Γ, Γ_{free}	0.175 , 0.222	DCC
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	R_{free} test set	1913 reflections (10.03%)	wwPDB-VP
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$ 0.33 , 55.3 EDS L-test for twinning² $< L > = 0.49, < L^2 > = 0.31$ Xtriage 0.016 for $-1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*l$ $3*k+1/3*l$ $3*k+1/3*l$ Xtriage Estimated twinning fraction $1/3*l,-4/3*h+4/3*l,-1/3*h-2/3*k+1/3*l$ Xtriage $1/3*l,-4/3*h+4/3*k+1/3*l$ 0.024 for $-h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k +1/3*l Fo,Fc correlation 0.97 EDS Total number of atoms 1671 wwPDB-VP $	Wilson B-factor (Å ²)	37.5	Xtriage
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		0.369	Xtriage
Estimated twinning fraction $ \begin{array}{c} 0.016 \text{ for } -1/3*\text{h} + 1/3*\text{k} + 1/3*\text{l}, -\text{k}, 8/3*\text{h} + 4/\\ 3*\text{k} + 1/3*\text{l}\\ 0.028 \text{ for } -2/3*\text{h} - 1/3*\text{k} - 1/3*\text{l}, -1/3*\text{h} - 2/3*\text{k} +\\ 1/3*\text{l}, -4/3*\text{h} + 4/3*\text{k} + 1/3*\text{l}\\ 0.024 \text{ for } -\text{h}, 1/3*\text{h} - 1/3*\text{k} - 1/3*\text{l}, -4/3*\text{h} - 8/3*\text{k}\\ +1/3*\text{l} \\ \hline \\ \text{Fo,F}_c \text{ correlation} \\ \hline \\ \text{Total number of atoms} \\ \end{array} \begin{array}{c} \text{EDS} \\ \text{wwPDB-VP} \\ \end{array} $	Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$		EDS
Estimated twinning fraction	L-test for twinning ²		Xtriage
Estimated twinning fraction			
$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$		3*k+1/3*l	
$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	Estimated twinning fraction		Xtriage
		$1/3^{+}1, -4/3^{+}h + 4/3^{+}k + 1/3^{+}1$	
F_o, F_c correlation 0.97 EDS Total number of atoms 1671 wwPDB-VP			
Total number of atoms 1671 wwPDB-VP	F _o .F _o correlation		EDS

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.78% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: K

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).

Mal	Chain	Bond	$\mathbf{lengths}$	Bond angles		
MOI		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	A	0.40	0/1587	0.59	0/2166	

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	1540	0	1477	9	1
2	A	1	0	0	0	0
3	A	130	0	0	1	0
All	All	1671	0	1477	9	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 3.

All (9) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} \text{Interatomic} \\ \text{distance (Å)} \end{array}$	Clash overlap (Å)
1:A:618:ARG:NH1	1:A:686:THR:OG1	2.40	0.54

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COMBINE	THOTH.	memous	DULUE.

Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	$\operatorname{distance} (\mathring{\mathbf{A}})$	overlap (Å)
1:A:702[B]:GLU:HG2	1:A:703:TYR:HD2	1.76	0.50
1:A:655:LEU:O	1:A:657:GLN:N	2.45	0.50
1:A:700:HIS:CE1	1:A:702[B]:GLU:HB3	2.46	0.50
1:A:572:ALA:O	1:A:576:LEU:HD12	2.17	0.44
1:A:618:ARG:NH1	1:A:686:THR:O	2.51	0.42
1:A:683:THR:OG1	3:A:901:HOH:O	2.09	0.42
1:A:657:GLN:HG2	1:A:658:GLU:H	1.86	0.41
1:A:683:THR:HB	1:A:685:ALA:H	1.86	0.40

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	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	Clash overlap (Å)
1:A:525:GLU:OE1	1:A:527:GLN:NE2[2_445]	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	lysed Favoured Allowed		Outliers	Percentiles
1	A	195/224 (87%)	186 (95%)	7 (4%)	2 (1%)	15 6

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	656	GLN
1	A	715	PRO

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	164/185 (89%)	163 (99%)	1 (1%)	86 87	

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	684	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



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>	# RSRZ > 2		$OWAB(Å^2)$	Q < 0.9
1	A	195/224 (87%)	0.12	11 (5%) 24	27	31, 49, 95, 145	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	576	LEU	6.9
1	A	655	LEU	6.1
1	A	577	PHE	4.4
1	A	656	GLN	4.3
1	A	654	ASP	3.4
1	A	716	ALA	3.4
1	A	578	GLY	3.2
1	A	575	SER	3.0
1	A	652	ASP	2.4
1	A	525	GLU	2.2
1	A	658	GLU	2.1

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)

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
2	K	A	801	1/1	1.00	0.10	33,33,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.

