



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2022 – 06:28 PM JST

PDB ID : 7F90
Title : Crystal structure of SARS auxiliary protein in complex with human nuclear protein
Authors : Gao, X.; Cui, S.
Deposited on : 2021-07-03
Resolution : 2.39 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	:	2.30
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)	:	2.30

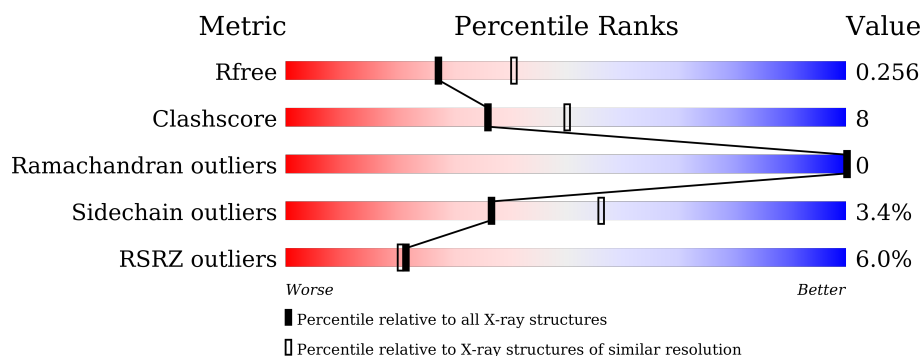
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	E	63	<div> <div>3%</div> <div> <div>11%</div> <div>5%</div> <div>84%</div> </div> </div>
1	F	63	<div> <div>10%</div> <div> <div>11%</div> <div>8%</div> <div>81%</div> </div> </div>
2	A	368	<div> <div>4%</div> <div> <div>73%</div> <div>15%</div> <div>11%</div> </div> </div>
2	C	368	<div> <div>2%</div> <div> <div>73%</div> <div>16%</div> <div>11%</div> </div> </div>
3	B	1817	<div> <div>0%</div> <div> <div>98%</div> </div> </div>
3	D	1817	<div> <div>0%</div> <div> <div>97%</div> </div> </div>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12124 atoms, of which 5832 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 ORF6 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	10	Total	C	H	N	O	S	0	0	0
			151	52	65	10	23	1			
1	F	12	Total	C	H	N	O	S	0	0	0
			162	63	61	12	25	1			

- Molecule 2 is a protein called mRNA export factor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	328	Total	C	H	N	O	S	0	0	0
			5096	1645	2499	452	483	17			
2	C	327	Total	C	H	N	O	S	0	1	0
			5086	1643	2494	449	483	17			

- Molecule 3 is a protein called Nuclear pore complex protein Nup98-Nup96.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	B	45	Total	C	H	N	O	S	0	0	0
			713	221	353	62	75	2			
3	D	46	Total	C	H	N	O	S	0	0	0
			727	225	360	63	77	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		
4	A	83	Total	O	0	0
			83	83		
4	C	90	Total	O	0	0
			90	90		

Continued on next page...

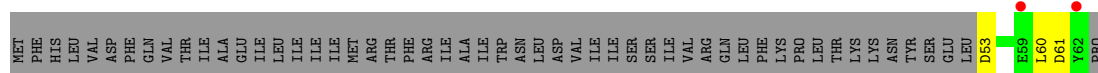
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	O	0	0
			5	5		
4	D	8	Total	O	0	0
			8	8		

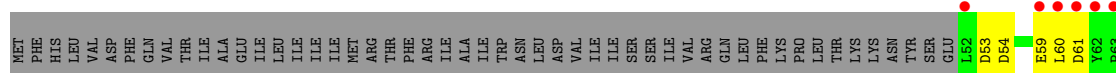
3 Residue-property plots

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.

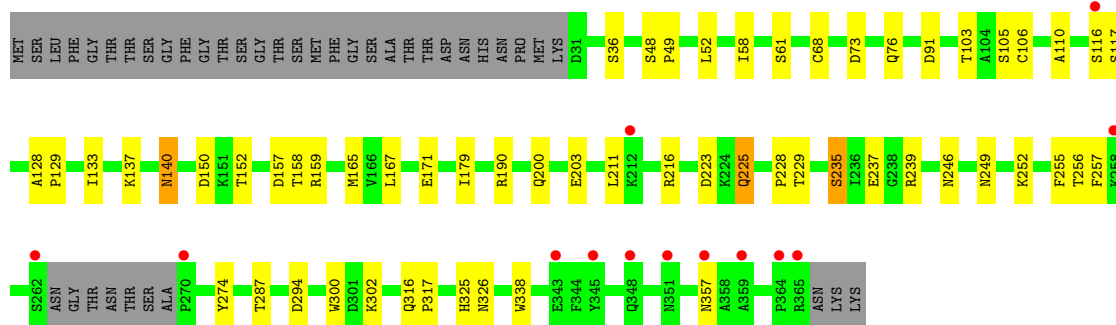
- Molecule 1: ORF6 protein



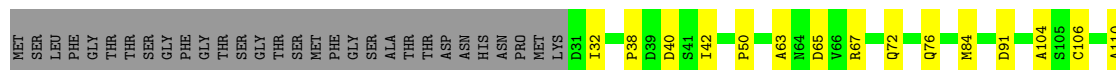
- Molecule 1: ORF6 protein



- Molecule 2: mRNA export factor



- Molecule 2: mRNA export factor







HIS	HIS	MET	HIS	VAL	TVR	TYR	LEU
PRO	PRO	ARG	ASN	ARG	ARG	ALA	ALA
ASP	HIS	ARG	ARG	LEU	LEU	CYS	GLY
ARG	CYS	ILE	CYS	LEU	TRP	PRO	LYS
THR	HIS	GLN	HIS	THR	HIS	LEU	VAL
THR	GLN	GLN	LEU	ARG	LEU	PRO	TRP
SER	VAL	ASP	LEU	HIS	TRP	SER	GLN
ASP	ASP	ASP	ILE	CYS	VAL	TYR	LEU
THR	SER	CYS	ARG	LEU	LEU	LEU	GLY
PRO	GLY	SER	HIS	LEU	ARG	GLY	LYS
ASP	ASN	ASN	LEU	GLU	ALA	SER	LYS
PRO	PRO	LEU	ALA	THR	LEU	GLY	GLN
ARG	GLN	ASP	SER	PRO	ASN	CYS	ILE
ARG	ARG	GLU	ASP	GLU	THR	VAL	ASN
VAL	VAL	GLN	ALA	SER	THR	ILE	VAL
PRO	PRO	LEU	ILE	TRP	HIS	ALA	CYS
ARG	HIS	ILE	ILE	ALA	LEU	GLU	SER
LEU	ARG	ILE	ASN	LYS	SER	GLY	GLN
LEU	LYS	GLU	GLU	GLU	ALA	GLN	LEU
LEU	LEU	VAL	ASN	THR	GLN	ASN	ASP
ALA	ALA	THR	TYR	PHE	CYS	SER	TRP
PRO	PRO	SER	ASP	LEU	GLU	GLN	LYS
HIS	HIS	LEU	TYR	THR	GLY	THR	ARG
ILE	ILE	CYS	LEU	GLN	VAL	PRO	SER
GLY	GLY	SER	LEU	GLY	LEU	LEU	LEU
ARG	ARG	ARG	GLY	LEU	GLN	ARG	ALA
LEU	LEU	ILE	PHE	ARG	ALA	ASP	ILE
PRO	PRO	GLU	LEU	VAL	SER	VAL	HIS
MET	MET	ILE	GLN	PRO	TYR	CYS	LEU
GLU	GLU	ILE	ASP	ALA	ALA	PHE	TRP
ASP	ASP	LYS	ARG	ALA	GLY	HIS	TYR
GLU	GLU	ASP	SER	LYS	GLY	SER	ALA
LEU	LEU	ARG	SER	ALA	LEU	ASP	ARG
ARG	ARG	LEU	LEU	VAL	TRP	ARG	ILE
SER	SER	ALA	ILE	ARG	GLU	HIS	SER
LEU	LEU	GLN	GLN	ALA	TRP	ARG	ARG
THR	THR	ASN	ASP	HIS	ALA	ASP	ALA
GLN	GLN	ASP	TRP	MET	ILE	LEU	SER
SER	SER	MET	GLU	GLU	PHE	ASN	SER
TYR	TYR	ALA	THR	SER	VAL	GLN	MET
LEU	LEU	LYS	SER	ASP	LEU	LEU	TYR
ARG	ARG	VAL	GLY	LYS	LEU	GLU	GLU
GLU	GLU	VAL	LEU	HIS	ILE	PRO	ALA
LEU	LEU	ALA	VAL	LEU	ARG	PHE	GLN
VAL	VAL	ASN	LEU	ALA	ASN	SER	ASN
GLY	GLY	LEU	LEU	LEU	SER	ILE	ASN
SER	SER	ARG	TYR	CYS	GLY	THR	THR
LEU	LEU	VAL	ILE	PHE	ASP	ASP	ASP
		VAL	ARG	VAL	GLY	PRO	SER
		LEU	VAL	LYS	GLU	ASP	LEU
		LEU	ILE	ALA	LYS	ASP	ARG
		THR	GLU	THR	ALA	ASP	ARG

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	189.33Å 86.79Å 47.91Å 90.00° 92.09° 90.00°	Depositor
Resolution (Å)	47.87 – 2.39 47.87 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.87-2.39) 99.9 (47.87-2.39)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.220 , 0.258 0.222 , 0.256	Depositor DCC
R_{free} test set	1603 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	31.2	Xtriage
Anisotropy	1.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.086 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12124	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [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	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	E	0.31	0/87	0.54	0/117
1	F	0.50	0/103	0.68	0/140
2	A	0.34	0/2672	0.57	1/3631 (0.0%)
2	C	0.32	0/2670	0.54	0/3629
3	B	0.26	0/364	0.47	0/487
3	D	0.27	0/371	0.51	0/497
All	All	0.32	0/6267	0.55	1/8501 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	190	ARG	NE-CZ-NH1	5.28	122.94	120.30

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	E	86	65	65	8	0
1	F	101	61	83	1	0
2	A	2597	2499	2499	39	0
2	C	2592	2494	2494	42	0
3	B	360	353	352	3	0
3	D	367	360	359	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	83	0	0	14	0
4	B	5	0	0	2	0
4	C	90	0	0	12	1
4	D	8	0	0	6	0
4	E	2	0	0	1	0
4	F	1	0	0	0	0
All	All	6292	5832	5852	95	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 8.

The worst 5 of 95 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)
2:A:246:ASN:OD1	4:A:401:HOH:O	1.83	0.95
2:C:76:GLN:OE1	4:C:401:HOH:O	1.85	0.95
2:C:220:ILE:O	4:C:402:HOH:O	1.88	0.91
1:E:61:ASP:OD1	2:A:239:ARG:NH1	2.05	0.89
2:A:150:ASP:OD1	2:A:152:THR:OG1	1.91	0.88

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)
4:C:411:HOH:O	4:C:437:HOH:O[2_556]	2.07	0.13

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	E	8/63 (13%)	8 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	10/63 (16%)	10 (100%)	0	0	100	100
2	A	324/368 (88%)	305 (94%)	19 (6%)	0	100	100
2	C	324/368 (88%)	311 (96%)	13 (4%)	0	100	100
3	B	41/1817 (2%)	41 (100%)	0	0	100	100
3	D	42/1817 (2%)	42 (100%)	0	0	100	100
All	All	749/4496 (17%)	717 (96%)	32 (4%)	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	E	10/61 (16%)	9 (90%)	1 (10%)	7	11
1	F	12/61 (20%)	8 (67%)	4 (33%)	0	0
2	A	285/317 (90%)	271 (95%)	14 (5%)	25	40
2	C	285/317 (90%)	281 (99%)	4 (1%)	67	82
3	B	41/1543 (3%)	41 (100%)	0	100	100
3	D	42/1543 (3%)	42 (100%)	0	100	100
All	All	675/3842 (18%)	652 (97%)	23 (3%)	37	56

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	235	SER
2	A	302	LYS
2	A	249	ASN
2	A	338	TRP
2	A	61	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	246	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	E	10/63 (15%)	1.57	2 (20%) 1 0	48, 57, 89, 92	0
1	F	12/63 (19%)	2.70	6 (50%) 0 0	44, 74, 100, 114	0
2	A	328/368 (89%)	0.69	13 (3%) 38 37	24, 36, 59, 89	0
2	C	327/368 (88%)	0.62	6 (1%) 68 66	22, 33, 53, 69	0
3	B	45/1817 (2%)	1.51	12 (26%) 0 0	35, 59, 77, 87	0
3	D	46/1817 (2%)	1.00	7 (15%) 2 1	31, 48, 67, 76	0
All	All	768/4496 (17%)	0.77	46 (5%) 21 20	22, 36, 65, 114	0

The worst 5 of 46 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	63	PRO	9.4
1	E	62	TYR	7.1
3	B	163	LYS	5.7
1	F	62	TYR	4.7
2	A	262	SER	4.7

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.