

Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 04:36 PM EDT

PDB ID : 4NJL

Title : Crystal structure of middle east respiratory syndrome coronavirus S2 protein

fusion core

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 $Deposited \ on \quad : \quad 2013\text{-}11\text{-}10$

Resolution : 2.30 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.orgA 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

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

Xtriage (Phenix) : 1.13 EDS : 2.35.1

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)

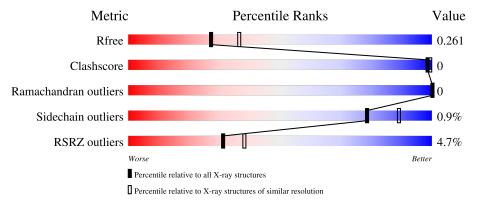
Validation Pipeline (wwPDB-VP) : 2.35.1

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 2.30 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 $(\# \mathrm{Entries})$	$\begin{array}{c} {\rm Similar\ resolution} \\ (\#{\rm Entries,\ resolution\ range(\mathring{A})}) \end{array}$
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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
		101	5%
1	A	131	97%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 1091 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 S protein.

\mathbf{Mol}	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	A	129	Total 980	C 610	N 166	O 201	S 3	0	1	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	983	SER	-	expression tag	UNP R9UQ53
A	1020	GLN	ARG	conflict	UNP R9UQ53
A	1064	SER	-	expression tag	UNP R9UQ53
A	1065	GLY	-	expression tag	UNP R9UQ53
A	1066	GLY	-	expression tag	UNP R9UQ53
A	1067	ARG	-	expression tag	UNP R9UQ53
A	1068	GLY	-	expression tag	UNP R9UQ53
A	1069	GLY	-	expression tag	UNP R9UQ53
A	1245	SER	-	expression tag	UNP R9UQ53
A	1246	ILE	-	expression tag	UNP R9UQ53
A	1247	PRO	-	expression tag	UNP R9UQ53
A	1248	ASN	-	expression tag	UNP R9UQ53
A	1249	PHE	-	expression tag	UNP R9UQ53
A	1250	GLY	-	expression tag	UNP R9UQ53
A	1251	SER	-	expression tag	UNP R9UQ53
A	1252	LEU	-	expression tag	UNP R9UQ53
A	1253	THR	-	expression tag	UNP R9UQ53
A	1254	GLN	_	expression tag	UNP R9UQ53
A	1255	ILE	-	expression tag	UNP R9UQ53
A	1256	ASN	-	expression tag	UNP R9UQ53
A	1257	THR	_	expression tag	UNP R9UQ53
A	1258	THR	-	expression tag	UNP R9UQ53
A	1259	LEU	_	expression tag	UNP R9UQ53
A	1260	LEU	-	expression tag	UNP R9UQ53
A	1261	ASP	-	expression tag	UNP R9UQ53
A	1262	LEU	-	expression tag	UNP R9UQ53
A	1263	THR	-	expression tag	UNP R9UQ53

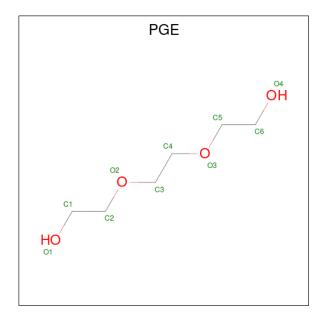
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Chain	Residue	Modelled	Actual	Comment	Reference
A	1264	TYR	-	expression tag	UNP R9UQ53
A	1265	GLU	-	expression tag	UNP R9UQ53
A	1266	MET	-	expression tag	UNP R9UQ53
A	1267	LEU	-	expression tag	UNP R9UQ53
A	1268	SER	-	expression tag	UNP R9UQ53
A	1269	LEU	-	expression tag	UNP R9UQ53
A	1270	GLN	-	expression tag	UNP R9UQ53
A	1271	GLN	-	expression tag	UNP R9UQ53
A	1272	VAL	-	expression tag	UNP R9UQ53
A	1273	VAL	-	expression tag	UNP R9UQ53
A	1274	LYS	-	expression tag	UNP R9UQ53
A	1275	ALA	-	expression tag	UNP R9UQ53
A	1276	LEU	-	expression tag	UNP R9UQ53
A	1277	ASN	-	expression tag	UNP R9UQ53
A	1278	GLU	-	expression tag	UNP R9UQ53
A	1279	SER	-	expression tag	UNP R9UQ53
A	1280	TYR	-	expression tag	UNP R9UQ53
A	1281	ILE	-	expression tag	UNP R9UQ53
A	1282	ASP	-	expression tag	UNP R9UQ53
A	1283	LEU	-	expression tag	UNP R9UQ53
A	1284	LYS		expression tag	UNP R9UQ53
A	1285	GLU	-	expression tag	UNP R9UQ53
A	1286	LEU	-	expression tag	UNP R9UQ53
A	1287	GLY	-	expression tag	UNP R9UQ53
A	1288	ASN	-	expression tag	UNP R9UQ53

 \bullet Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $\mathrm{C_6H_{14}O_4}).$





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0

• Molecule 3 is water.

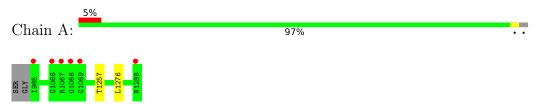
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	101	Total O 101 101	0	0



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: S protein





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants	43.51Å 43.51Å 129.63Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.18 - 2.30	Depositor
Resolution (A)	36.18 - 2.20	EDS
% Data completeness	99.3 (36.18-2.30)	Depositor
(in resolution range)	88.9 (36.18-2.20)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.50 (at 2.20Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
P.P.	0.220 , 0.261	Depositor
R, R_{free}	0.220 , 0.261	DCC
R_{free} test set	384 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.32 , 38.0	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.079 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	1091	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 12.52% 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: PGE

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	0.23	0/990	0.38	0/1337	

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	980	0	988	1	0
2	A	10	0	14	0	0
3	A	101	0	0	0	0
All	All	1091	0	1002	1	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 0.

All (1) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} \ ({\rm \AA}) \end{array}$	$egin{aligned} \operatorname{Clash} \ \operatorname{overlap}\ (\begin{subarray}{c} \begin{subarray}{c} \begi$
1:A:1276:LEU:HA	1:A:1276:LEU:HD23	1.84	0.41



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	Percentiles
1	A	128/131 (98%)	128 (100%)	0	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	Analysed Rotameric		Percentiles	
1	A	109/109 (100%)	108 (99%)	1 (1%)	78 89	

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

Mol	Chain	Res	Type
1	A	1257	THR

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)

1 ligand is 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	Mol Type Chain		n Res Linl	Link	Bond lengths			Bond angles		
MIOI	Type	Chain	nes .	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PGE	A	2001	-	9,9,9	0.30	0	8,8,8	0.31	0

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.

\mathbf{Mol}	\mathbf{Type}	Chain	Res	Link	$\mathbf{Chirals}$	Torsions	Rings
2	PGE	A	2001	-	ı	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2001	PGE	O3-C5-C6-O4

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 $>$	$\# \mathrm{RSRZ} {>} 2$	$OWAB(A^2)$	Q < 0.9
1	A	129/131 (98%)	-0.20	6 (4%) 31 38	24, 36, 84, 122	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1068	GLY	4.8
1	A	1067	ARG	3.3
1	A	1288	ASN	2.7
1	A	985	ILE	2.3
1	A	1066	GLY	2.2
1	A	1069	GLY	2.0

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	${f B-factors}({f \AA}^2)$	Q<0.9
2	PGE	A	2001	10/10	0.75	0.15	65,75,86,87	0



6.5 Other polymers (i)

There are no such residues in this entry.

