wwPDB X-ray Structure Validation Summary Report (i)

Feb 18, 2023 – 08:03 am GMT

PDB ID	:	7ZR2
Title	:	Crystal structure of a chimeric protein mimic of SARS-CoV-2 Spike HR1 in complex with HR2
Authors	:	Camara-Artigas, A.; Gavira, J.A.; Cano-Munoz, M.; Polo-Megias, D.; Conejero-Lara, F.
Deposited on	:	2022-05-03
Resolution	:	1.45 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

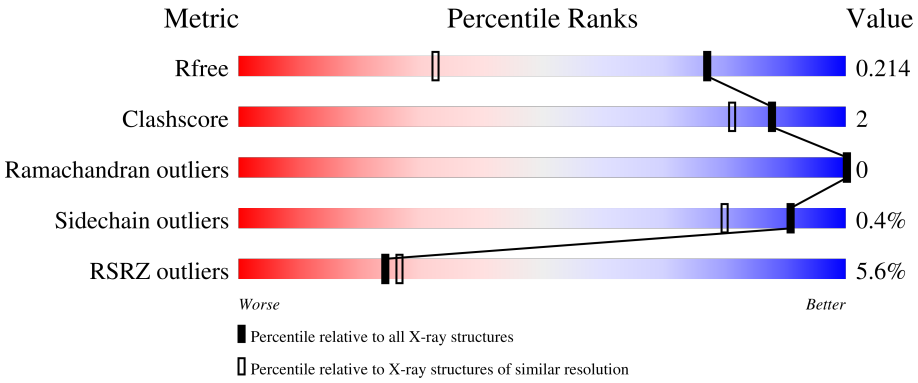
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 1.45 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	1156 (1.46-1.46)
Clashscore	141614	1202 (1.46-1.46)
Ramachandran outliers	138981	1178 (1.46-1.46)
Sidechain outliers	138945	1178 (1.46-1.46)
RSRZ outliers	127900	1139 (1.46-1.46)

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	241	6%, 91%, 6%
2	B	44	2%, 91%, 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4350 atoms, of which 2020 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 Spike protein S2',Chimeric protein mimic of SARS-CoV-2 Spike HR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	A	227	3444	1063	1721	306	354	0	2	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P0DTC2
A	1	ASP	ASN	engineered mutation	UNP P0DTC2
A	13	LYS	GLN	engineered mutation	UNP P0DTC2
A	31	GLU	ALA	engineered mutation	UNP P0DTC2
A	38	GLU	VAL	engineered mutation	UNP P0DTC2
A	45	ASP	ALA	engineered mutation	UNP P0DTC2
A	59	ARG	ALA	engineered mutation	UNP P0DTC2
A	63	GLU	VAL	engineered mutation	UNP P0DTC2
A	165	GLU	ALA	engineered mutation	UNP P0DTC2
A	183	LYS	ALA	engineered mutation	UNP P0DTC2
A	190	LYS	GLN	engineered mutation	UNP P0DTC2
A	197	LYS	ALA	engineered mutation	UNP P0DTC2
A	222	LYS	LEU	engineered mutation	UNP P0DTC2
A	230	GLY	-	expression tag	UNP P0DTC2
A	231	GLY	-	expression tag	UNP P0DTC2
A	232	GLY	-	expression tag	UNP P0DTC2
A	233	GLY	-	expression tag	UNP P0DTC2
A	234	SER	-	expression tag	UNP P0DTC2
A	235	HIS	-	expression tag	UNP P0DTC2
A	236	HIS	-	expression tag	UNP P0DTC2
A	237	HIS	-	expression tag	UNP P0DTC2
A	238	HIS	-	expression tag	UNP P0DTC2
A	239	HIS	-	expression tag	UNP P0DTC2
A	240	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called Spike protein S2'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	41	Total	C	H	N	O	0	0	0
			602	186	299	52	65			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1163	ACE	ASP	conflict	UNP P0DTC2
B	1203	SER	LEU	conflict	UNP P0DTC2
B	1205	GLY	LYS	conflict	UNP P0DTC2

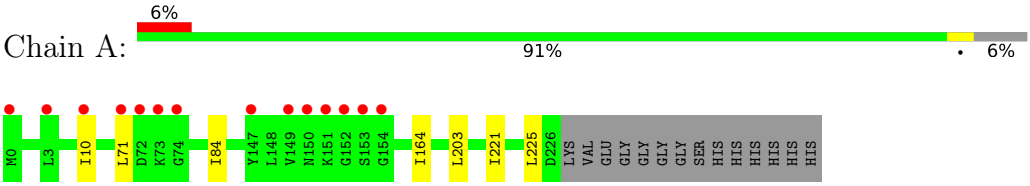
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	243	Total	O	0	0
			243	243		
3	B	61	Total	O	0	0
			61	61		

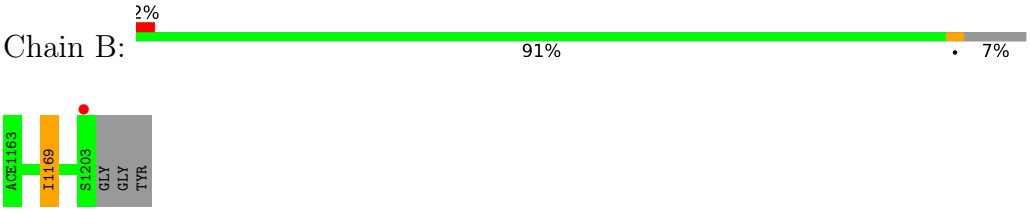
3 Residue-property plots (i)

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: Spike protein S2',Chimeric protein mimic of SARS-CoV-2 Spike HR1



• Molecule 2: Spike protein S2'



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.78Å 37.37Å 43.91Å 90.00° 95.67° 90.00°	Depositor
Resolution (Å)	18.80 – 1.45 18.92 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.0 (18.80-1.45) 96.0 (18.92-1.45)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.72 (at 1.45Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.174 , 0.209 0.178 , 0.214	Depositor DCC
R_{free} test set	2266 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	15.1	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 45.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4350	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.15% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/1732	0.48	0/2331
2	B	0.43	0/300	0.58	0/406
All	All	0.40	0/2032	0.49	0/2737

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

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	1723	1721	1722	8	0
2	B	303	299	303	1	0
3	A	243	0	0	0	0
3	B	61	0	0	0	0
All	All	2330	2020	2025	8	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 2.

The worst 5 of 8 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:A:10:ILE:HD11	1:A:164:ILE:HD13	1.55	0.87
1:A:84:ILE:HD12	1:A:225:LEU:HD11	1.67	0.75
1:A:10:ILE:CD1	1:A:164:ILE:HD13	2.27	0.61
1:A:84:ILE:HD13	1:A:221:ILE:HG22	1.93	0.51
1:A:84:ILE:CD1	1:A:225:LEU:HD11	2.39	0.49

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	227/241 (94%)	225 (99%)	2 (1%)	0	100	100
2	B	39/44 (89%)	39 (100%)	0	0	100	100
All	All	266/285 (93%)	264 (99%)	2 (1%)	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	Outliers	Percentiles	
1	A	191/213 (90%)	191 (100%)	0	100	100
2	B	34/37 (92%)	33 (97%)	1 (3%)	42	10
All	All	225/250 (90%)	224 (100%)	1 (0%)	91	80

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

Mol	Chain	Res	Type
2	B	1169	ILE

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	227/241 (94%)	0.17	14 (6%) 20 22	11, 21, 40, 57	0
2	B	40/44 (90%)	-0.23	1 (2%) 57 60	12, 20, 33, 37	0
All	All	267/285 (93%)	0.11	15 (5%) 24 26	11, 21, 40, 57	0

The worst 5 of 15 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	153	SER	7.3
1	A	149	VAL	7.0
1	A	154	GLY	6.4
1	A	72	ASP	5.7
1	A	150	ASN	5.4

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.