

wwPDB X-ray Structure Validation Summary Report (i)

Jan 10, 2022 – 12:22 pm GMT

PDB ID : 7QNX

Title: The receptor binding domain of SARS-CoV-2 spike glycoprotein in complex

with Beta-55 and EY6A Fabs

Authors : Zhou, D.; Ren, J.; Stuart, D.I.

Deposited on : 2021-12-23

Resolution : 2.92 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467

Mogul : 1.8.4, CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.24

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

Refmac: 5.8.0267

CCP4 : 7.1.010 (Gargrove)

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

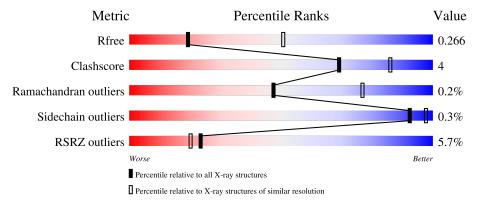
Validation Pipeline (wwPDB-VP) : 2.24

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 2.92 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 $(\#\text{Entries})$	Similar resolution $(\#\text{Entries, resolution range}(\mathring{A}))$
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	
1	Н	226	5% 81%	13% 5%
2	L	215	92%	7% •
3	A	232	6% 87%	11% •
4	В	215	93%	6%
5	Е	202	13%	10% 8%

Continued on next page...



Continued from previous page...

Mol	Chain	Length	Quality of chain
6	С	2	100%



2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8125 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 EY6A heavy chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Н	215	Total 1637	C 1041	N 273	O 317	S 6	0	0	0

• Molecule 2 is a protein called EY6A light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
2	Т	212	Total	С	N	О	S	0	0	0
2		212	1618	1012	270	331	5			

• Molecule 3 is a protein called Beta-55 heavy chain.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
3	A	228	Total 1720	C 1097	N 279	O 339	S 5	0	0	0

• Molecule 4 is a protein called Beta-55 light chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
4	В	214	Total 1645	C 1033	N 277	O 330	S 5	0	0	0

• Molecule 5 is a protein called Surface glycoprotein.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
5	Е	185	Total 1477	C 947	N 245	O 278	S 7	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

	Chain	Residue	Modelled	Actual	Comment	Reference
	Ε	327	HIS	-	expression tag	UNP A0A894R379
ĺ	Ε	328	HIS	-	expression tag	UNP A0A894R379

Continued on next page...



 $Continued\ from\ previous\ page...$

Chain	Residue	Modelled	Actual	Comment	Reference
Е	329	HIS	-	expression tag	UNP A0A894R379
Е	330	HIS	-	expression tag	UNP A0A894R379
E	331	HIS	-	expression tag	UNP A0A894R379
Е	332	HIS	-	expression tag	UNP A0A894R379
E	527	LYS	PRO	variant	UNP A0A894R379

 \bullet Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



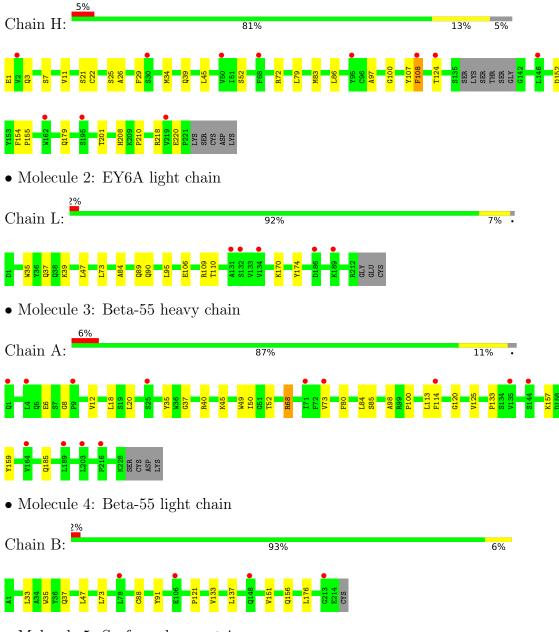
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	С	2	Total C N O 28 16 2 10	0	0	0



3 Residue-property plots (i)

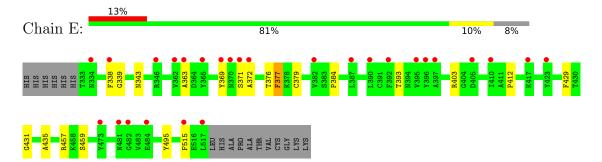
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: EY6A heavy chain



• Molecule 5: Surface glycoprotein





 \bullet Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	131.77Å 131.77Å 116.84Å	Donositon
a, b, c, α , β , γ	90.00° 90.00° 120.00°	Depositor
Resolution (Å)	81.64 - 2.92	Depositor
Resolution (A)	81.64 - 2.92	EDS
% Data completeness	99.7 (81.64-2.92)	Depositor
(in resolution range)	99.6 (81.64-2.92)	EDS
R_{merge}	0.55	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.03 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
D D.	0.229 , 0.266	Depositor
R, R_{free}	0.230 , 0.266	DCC
R_{free} test set	1236 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	69.2	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L > = 0.44, < L^2> = 0.27$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8125	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.74% 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: NAG

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	Н	0.24	0/1679	0.48	0/2288	
2	L	0.25	0/1651	0.47	0/2241	
3	A	0.25	0/1768	0.48	0/2419	
4	В	0.25	0/1682	0.48	0/2284	
5	Е	0.26	0/1518	0.47	0/2064	
All	All	0.25	0/8298	0.48	0/11296	

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	Н	1637	0	1591	18	0
2	L	1618	0	1582	8	0
3	A	1720	0	1684	17	0
4	В	1645	0	1608	8	0
5	Е	1477	0	1395	11	0
6	С	28	0	25	0	0
All	All	8125	0	7885	59	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.

The worst 5 of 59 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)	
3:A:49:TRP:HE1	3:A:52:THR:HG23	1.56	0.71	
1:H:29:PHE:O	1:H:72:ARG:NH2	2.34	0.61	
3:A:35:TYR:HB2	3:A:100:PRO:HG2	1.82	0.61	
3:A:133:PRO:HB3	3:A:159:TYR:HB3	1.86	0.57	
1:H:97:ALA:HB1	1:H:108:PHE:HB3	1.86	0.57	

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	Н	211/226 (93%)	202 (96%)	9 (4%)	0	100	100
2	L	210/215 (98%)	203 (97%)	7 (3%)	0	100	100
3	A	$226/232 \ (97\%)$	215 (95%)	11 (5%)	0	100	100
4	В	212/215 (99%)	204 (96%)	8 (4%)	0	100	100
5	E	183/202 (91%)	171 (93%)	10 (6%)	2 (1%)	14	41
All	All	1042/1090 (96%)	995 (96%)	45 (4%)	2 (0%)	47	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type	
5 E		372	ALA	
5	Е	371	SER	



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	Н	181/191 (95%)	180 (99%)	1 (1%)	86	95	
2	L	186/188 (99%)	186 (100%)	0	100	100	
3	A	197/202 (98%)	196 (100%)	1 (0%)	88	96	
4	В	186/187 (100%)	186 (100%)	0	100	100	
5	E	161/175 (92%)	160 (99%)	1 (1%)	86	95	
All	All	911/943 (97%)	908 (100%)	3 (0%)	92	98	

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Н	108	PHE
3	A	68	ARG
5	Е	377	PHE

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)

2 monosaccharides 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	Trino	Chain	Dag	Link	Bond lengths			Bond angles		
		Type	Chain	Res	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
	6	NAG	С	1	6,5	14,14,15	0.39	0	17,19,21	0.48	0
	6	NAG	С	2	6	14,14,15	0.25	0	17,19,21	0.46	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.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	С	1	6,5	-	0/6/23/26	0/1/1/1
6	NAG	С	2	6	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

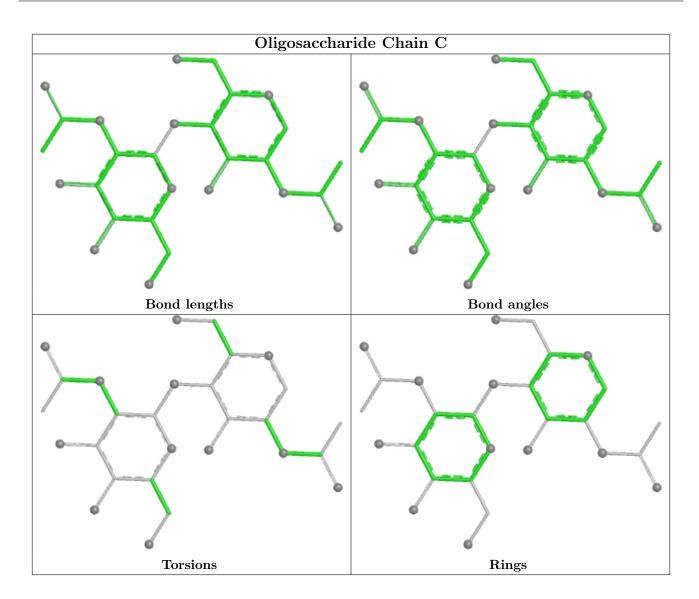
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





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></rsrz>	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	Н	215/226 (95%)	0.48	11 (5%) 28 24	60, 78, 105, 132	0
2	L	212/215 (98%)	0.42	5 (2%) 59 57	55, 70, 99, 149	0
3	A	228/232 (98%)	0.42	13 (5%) 23 20	51, 67, 107, 139	0
4	В	214/215 (99%)	0.39	4 (1%) 66 65	54, 71, 93, 122	0
5	E	185/202 (91%)	0.98	27 (14%) 2 1	56, 71, 115, 155	0
All	All	1054/1090 (96%)	0.53	60 (5%) 23 20	51, 71, 105, 155	0

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ	
5	Е	517	LEU	5.6	
5	Е	482	GLY	5.4	
3	A	1	GLN	5.0	
2	L	189	LYS	4.9	
5 E		371	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)

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.

\mathbf{Mol}	\mathbf{Type}	Chain	Res	Atoms	RSCC	RSR	$\operatorname{B-factors}(\mathrm{\AA}^2)$	Q<0.9
6	NAG	С	2	14/15	0.79	0.29	121,127,133,133	0

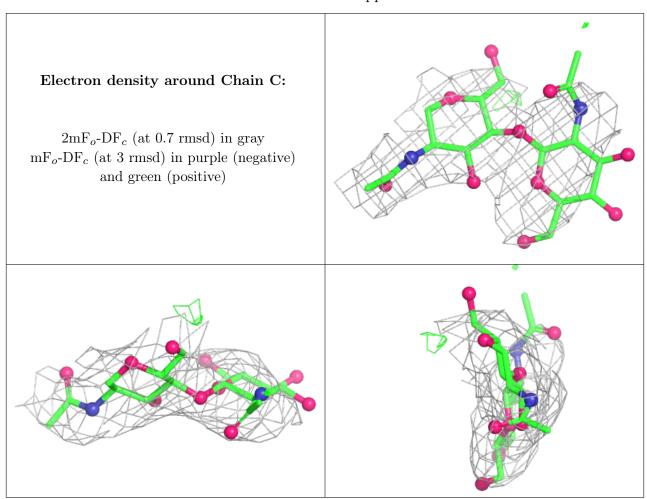
Continued on next page...



Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
6	NAG	С	1	14/15	0.86	0.20	90,111,117,123	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

