



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 9, 2021 – 08:11 am GMT

PDB ID : 6ZLR  
Title : Soaking competent crystal form of the SARS-CoV-2 Receptor Binding Domain (RBD):CR3022 complex.  
Authors : de Nicola, G.F.; Nichols, C.E.  
Deposited on : 2020-07-01  
Resolution : 3.10 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](mailto: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.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
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)	:	2.16

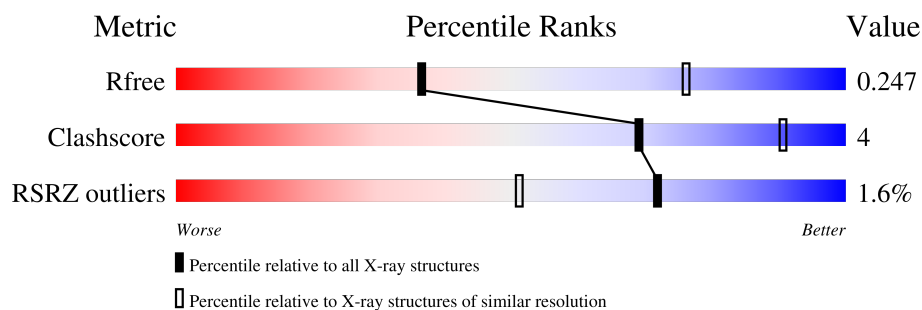
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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 <sub>free</sub>	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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  $\geq 3$ , 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	AAA	231	<div> <div>3%</div> <div>77%</div> <div>7%</div> <div>15%</div> </div>
1	DDD	231	<div> <div>3%</div> <div>79%</div> <div>6%</div> <div>15%</div> </div>
1	EEE	231	<div> <div>4%</div> <div>78%</div> <div>6%</div> <div>15%</div> </div>
2	BBB	222	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
2	FFF	222	<div> <div>%</div> <div>91%</div> <div>9%</div> </div>
2	HHH	222	<div> <div>2%</div> <div>92%</div> <div>8%</div> </div>
3	CCC	221	<div> <div>93%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	GGG	221	<div><div></div><div>95%</div><div></div></div>
3	LLL	221	<div><div></div><div>93%</div><div>6%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14736 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	EEE	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			
1	AAA	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			
1	DDD	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EEE	542	SER	-	expression tag	UNP P0DTC2
EEE	543	GLY	-	expression tag	UNP P0DTC2
EEE	544	HIS	-	expression tag	UNP P0DTC2
EEE	545	HIS	-	expression tag	UNP P0DTC2
EEE	546	HIS	-	expression tag	UNP P0DTC2
EEE	547	HIS	-	expression tag	UNP P0DTC2
EEE	548	HIS	-	expression tag	UNP P0DTC2
EEE	549	HIS	-	expression tag	UNP P0DTC2
AAA	542	SER	-	expression tag	UNP P0DTC2
AAA	543	GLY	-	expression tag	UNP P0DTC2
AAA	544	HIS	-	expression tag	UNP P0DTC2
AAA	545	HIS	-	expression tag	UNP P0DTC2
AAA	546	HIS	-	expression tag	UNP P0DTC2
AAA	547	HIS	-	expression tag	UNP P0DTC2
AAA	548	HIS	-	expression tag	UNP P0DTC2
AAA	549	HIS	-	expression tag	UNP P0DTC2
DDD	542	SER	-	expression tag	UNP P0DTC2
DDD	543	GLY	-	expression tag	UNP P0DTC2
DDD	544	HIS	-	expression tag	UNP P0DTC2
DDD	545	HIS	-	expression tag	UNP P0DTC2
DDD	546	HIS	-	expression tag	UNP P0DTC2
DDD	547	HIS	-	expression tag	UNP P0DTC2
DDD	548	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	549	HIS	-	expression tag	UNP P0DTC2

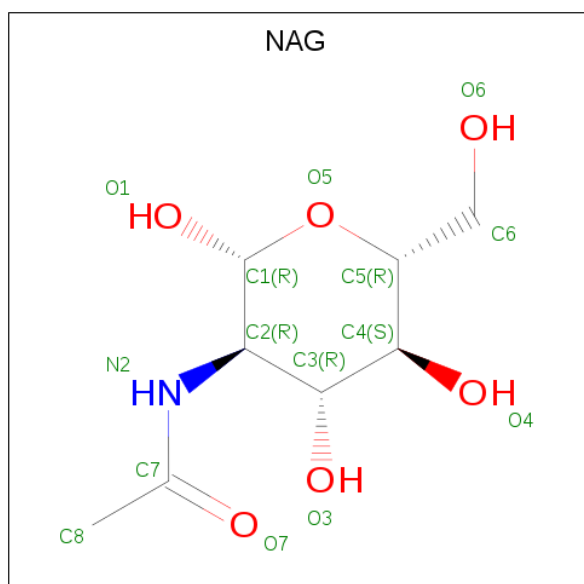
- Molecule 2 is a protein called CR3022 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	HHH	222	Total	C	N	O	S	0	0	0
			1647	1043	268	327	9			
2	BBB	222	Total	C	N	O	S	0	0	0
			1647	1043	268	327	9			
2	FFF	222	Total	C	N	O	S	0	0	0
			1647	1043	268	327	9			

- Molecule 3 is a protein called CR3022 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	LLL	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			
3	CCC	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			
3	GGG	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

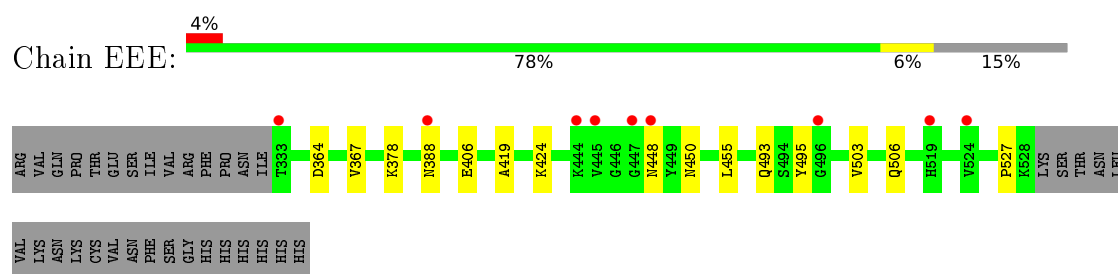


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	EEE	1	Total	C	N	O	0	0
			14	8	1	5		
4	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
4	DDD	1	Total	C	N	O	0	0
			14	8	1	5		

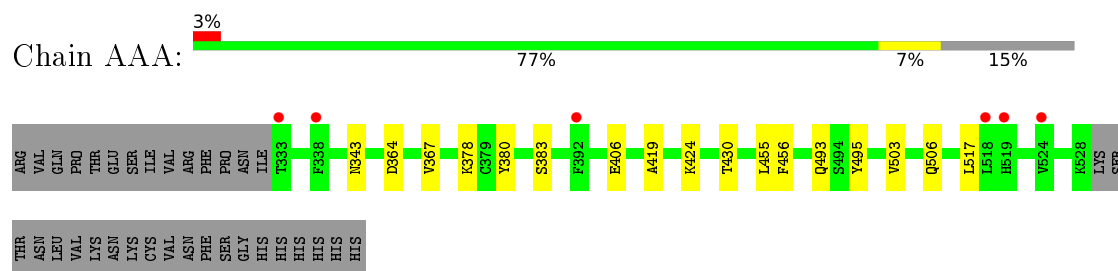
### 3 Residue-property plots [i](#)

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.

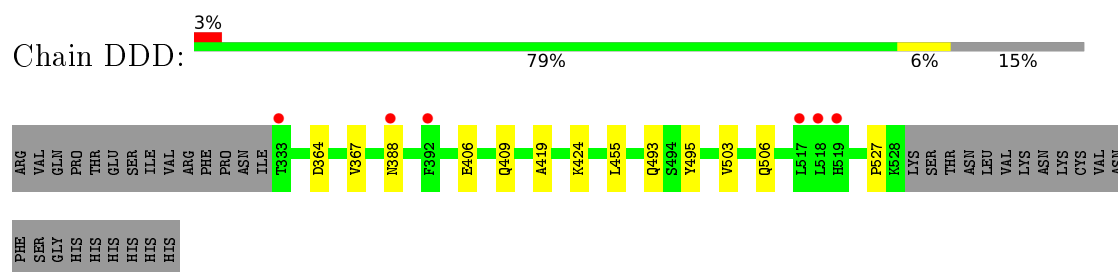
- Molecule 1: Spike glycoprotein



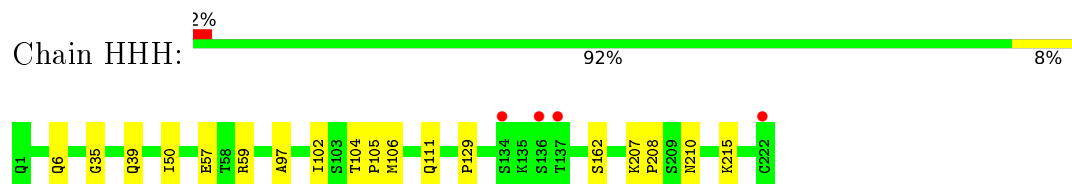
- Molecule 1: Spike glycoprotein



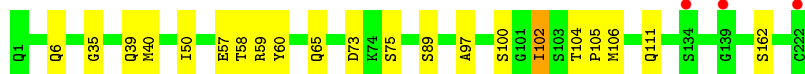
- Molecule 1: Spike glycoprotein



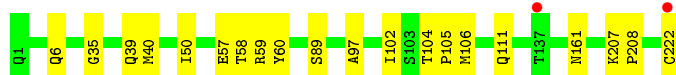
- Molecule 2: CR3022 FAB HEAVY CHAIN



- Molecule 2: CR3022 FAB HEAVY CHAIN



- Molecule 2: CR3022 FAB HEAVY CHAIN



- Molecule 3: CR3022 FAB LIGHT CHAIN



- Molecule 3: CR3022 FAB LIGHT CHAIN



- Molecule 3: CR3022 FAB LIGHT CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	207.13Å 207.13Å 199.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.03 – 3.10 67.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.5 (68.03-3.10) 90.5 (67.94-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.218 , 0.247 0.217 , 0.247	Depositor DCC
$R_{free}$ test set	3669 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 28.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.001 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	14736	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

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	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	AAA	0.68	0/1592	0.85	0/2168
1	DDD	0.67	0/1592	0.84	0/2168
1	EEE	0.66	0/1592	0.82	0/2168
2	BBB	0.68	0/1689	0.89	1/2299 (0.0%)
2	FFF	0.67	0/1689	0.88	0/2299
2	HHH	0.67	0/1689	0.89	0/2299
3	CCC	0.67	0/1741	0.87	1/2367 (0.0%)
3	GGG	0.65	0/1741	0.86	1/2367 (0.0%)
3	LLL	0.67	0/1741	0.87	0/2367
All	All	0.67	0/15066	0.86	3/20502 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GGG	148	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	CCC	148	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	BBB	102	ILE	N-CA-C	-5.04	97.39	111.00

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	AAA	1548	0	1462	18	0
1	DDD	1548	0	1460	7	0
1	EEE	1548	0	1461	9	0
2	BBB	1647	0	1623	21	0
2	FFF	1647	0	1623	18	0
2	HHH	1647	0	1623	17	0
3	CCC	1703	0	1649	16	0
3	GGG	1703	0	1649	12	0
3	LLL	1703	0	1649	13	0
4	AAA	14	0	13	4	0
4	DDD	14	0	13	0	0
4	EEE	14	0	13	1	0
All	All	14736	0	14238	106	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 106 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:AAA:343:ASN:HD21	4:AAA:601:NAG:C1	1.31	1.38
1:AAA:343:ASN:ND2	4:AAA:601:NAG:C1	1.93	1.29
2:FFF:39:GLN:HE22	3:GGG:44:GLN:HE22	1.02	0.94
2:BBB:39:GLN:HE22	3:CCC:44:GLN:HE22	1.11	0.93
2:HHH:39:GLN:HE22	3:LLL:44:GLN:HE22	1.21	0.89

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

### 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](#)

3 ligands are modelled in this entry.

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AAA	196/231 (84%)	0.04	6 (3%)	49	26	36, 65, 120, 143	0
1	DDD	196/231 (84%)	0.03	6 (3%)	49	26	33, 61, 116, 153	0
1	EEE	196/231 (84%)	0.42	9 (4%)	32	16	39, 95, 142, 165	0
2	BBB	222/222 (100%)	-0.18	3 (1%)	75	56	27, 47, 79, 143	0
2	FFF	222/222 (100%)	-0.17	2 (0%)	84	69	28, 48, 82, 203	0
2	HHH	222/222 (100%)	-0.19	4 (1%)	68	47	26, 45, 88, 161	0
3	CCC	219/221 (99%)	-0.31	0	100	100	31, 51, 76, 98	0
3	GGG	219/221 (99%)	-0.19	1 (0%)	91	81	33, 57, 90, 103	0
3	LLL	219/221 (99%)	-0.28	0	100	100	32, 54, 79, 115	0
All	All	1911/2022 (94%)	-0.10	31 (1%)	72	51	26, 54, 114, 203	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	FFF	222	CYS	7.0
1	EEE	333	THR	5.6
2	HHH	222	CYS	5.1
1	DDD	333	THR	3.6
2	BBB	222	CYS	3.6

### 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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	AAA	601	14/15	0.73	0.22	80,110,124,124	0
4	NAG	EEE	601	14/15	0.80	0.31	77,128,145,155	0
4	NAG	DDD	601	14/15	0.84	0.23	76,107,112,112	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.