

# wwPDB X-ray Structure Validation Summary Report (i)

Jan 15, 2024 – 11:54 am GMT

PDB ID : 6Z2M

Title : H11-D4, SARS-CoV-2 RBD, CR3022 ternary complex Authors : Naismith, J.H.; Ren, J.; Zhou, D.; Zhao, Y.; Stuart, D.I.

Deposited on : 2020-05-17

Resolution : 2.71 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 (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 : 2.36

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)

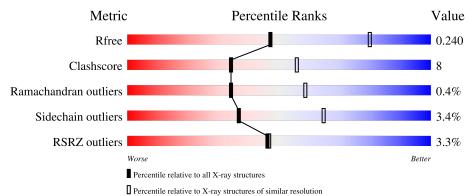
Validation Pipeline (wwPDB-VP) : 2.36

# 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 2.71 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	$\begin{array}{c} \text{Whole archive} \\ (\#\text{Entries}) \end{array}$	Similar resolution $(\#\text{Entries, resolution range}(\text{Å}))$		
$R_{free}$	130704	3359 (2.74-2.70)		
Clashscore	141614	3686 (2.74-2.70)		
Ramachandran outliers	138981	3622 (2.74-2.70)		
Sidechain outliers	138945	3623 (2.74-2.70)		
RSRZ outliers	127900	3276 (2.74-2.70)		

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		
		10=	5%		
1	A	197	69%	28%	•
			4%		
1	E	197	81%	17%	••
			3%		
2	В	216	79%	19%	•
			2%		
2	Н	216	84%	16%	
			% -		
3	С	219	78%	21%	•

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Mol	Chain	Length	Quality of chain		
3	L	219	80%	19%	<del>-</del> -
4	D	127	84%	15%	
4	F	127	79%	20%	•



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11731 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	A	197	Total 1560	C 1001	N 260	O 291	S 8	0	0	0
1	Е	195	Total 1543	С	N 257	O 289	S 8	0	0	0

• Molecule 2 is a protein called CR3022 antibody.

Mol	Chain	Residues		Ato	oms			ZeroOcc	AltConf	Trace
2	9 B	216	Total	С	N	О	S	0	1	0
	D	210	1609	1023	261	317	8		1	
2	П	216	Total	С	N	О	S	0	1	0
	216	1609	1023	261	317	8	0	1		

• Molecule 3 is a protein called CR3022 antibody.

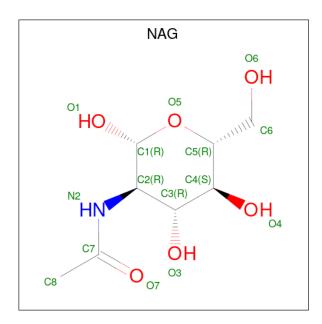
Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace
3	С	219	Total 1703	C 1070	- '	O 347	S 4	0	0	0
3	L	219	Total 1703	C 1070		O 347	S 4	0	0	0

• Molecule 4 is a protein called nanobody D4.

Mol	Chain	Residues		Atoms			ZeroOcc	AltConf	Trace	
4	Г	127	Total	С	N	О	S	0	0	0
4 F	121	988	621	173	189	5	0	0	0	
1	D	127	Total	С	N	О	S	0	0	0
4	4 D	121	988	621	173	189	5	U	0	U

• Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).





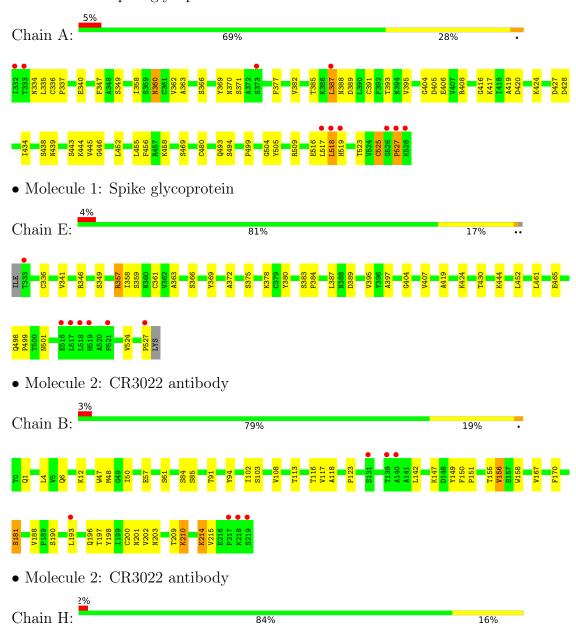
Mol	Chain	Residues					ZeroOcc	AltConf
5	A	1	Total 14				0	0
5	Е	1	Total 14	C 8	N 1	O 5	0	0



# 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: Spike glycoprotein









# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	149.72Å 150.40Å 119.54Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	74.86 - 2.71	Depositor
Resolution (A)	74.86 - 2.71	EDS
% Data completeness	64.3 (74.86-2.71)	Depositor
(in resolution range)	64.3 (74.86 - 2.71)	EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	1.48 (at 2.73Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
Ρ. Р.	0.198 , 0.241	Depositor
$R, R_{free}$	0.198 , $0.240$	DCC
$R_{free}$ test set	2365 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.7	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.27 , 24.1	EDS
L-test for twinning <sup>2</sup>	$< L > = 0.48, < L^2> = 0.31$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	11731	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>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.



<sup>&</sup>lt;sup>1</sup>Intensities 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			
MIOI	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5		
1	A	0.32	0/1604	0.54	1/2183~(0.0%)		
1	Е	0.32	0/1587	0.49	0/2161		
2	В	0.30	0/1654	0.54	0/2253		
2	Н	0.30	0/1654	0.50	0/2253		
3	С	0.31	0/1741	0.50	0/2367		
3	L	0.30	0/1741	0.50	0/2367		
4	D	0.29	0/1010	0.51	0/1366		
4	F	0.28	0/1010	0.51	0/1366		
All	All	0.30	0/12001	0.51	1/16316 (0.0%)		

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	С	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	$\mathbf{Z}$	$\mathbf{Observed}(^{o})$	$\operatorname{Ideal}({}^o)$
1	A	505	TYR	C-N-CA	6.02	136.76	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	С	171	GLU	Peptide



#### 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	1560	0	1483	43	0
1	Е	1543	0	1459	22	0
2	В	1609	0	1585	36	0
2	Н	1609	0	1585	23	0
3	С	1703	0	1649	37	0
3	L	1703	0	1649	26	1
4	D	988	0	951	10	0
4	F	988	0	951	17	1
5	A	14	0	13	0	0
5	Е	14	0	13	0	0
All	All	11731	0	11338	194	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 194 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$egin{aligned}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{aligned}$	$\begin{array}{c} \text{Clash} \\ \text{overlap } (\text{\AA}) \end{array}$
2:B:198:TYR:H	2:B:214:LYS:HE2	1.09	1.08
2:B:214:LYS:NZ	2:B:215:VAL:O	2.01	0.91
2:B:198:TYR:N	2:B:214:LYS:HE2	1.87	0.88
4:D:13:GLN:HG2	4:D:126:SER:HB2	1.59	0.84
2:B:91:THR:HG23	2:B:116:THR:HA	1.67	0.77

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-1 Atom-2		$egin{aligned}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{aligned}$
3:L:14:SER:OG	4:F:127:SER:OG[1_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	Perce	entiles
1	A	195/197 (99%)	175 (90%)	17 (9%)	3 (2%)	10	24
1	E	193/197 (98%)	176 (91%)	17 (9%)	0	100	100
2	В	213/216 (99%)	203 (95%)	9 (4%)	1 (0%)	29	53
2	Н	213/216 (99%)	204 (96%)	9 (4%)	0	100	100
3	С	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
3	L	217/219 (99%)	207 (95%)	10 (5%)	0	100	100
4	D	125/127 (98%)	123 (98%)	1 (1%)	1 (1%)	19	41
4	F	125/127 (98%)	123 (98%)	1 (1%)	1 (1%)	19	41
All	All	1498/1518 (99%)	1418 (95%)	74 (5%)	6 (0%)	34	58

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	27	ARG
1	A	360	ASN
1	A	518	LEU
4	F	27	ARG
1	A	527	PRO

#### 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	170/170 (100%)	161 (95%)	9 (5%)	22 46

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Mol	Chain	Chain Analysed Rotameric Outliers		Percentiles		
1	E	168/170~(99%)	165 (98%)	3 (2%)	59	82
2	В	$182/181\ (101\%)$	175 (96%)	7 (4%)	33	60
2	Н	182/181 (101%)	178 (98%)	4 (2%)	52	78
3	С	$194/194\ (100\%)$	186 (96%)	8 (4%)	30	57
3	L	$194/194\ (100\%)$	188 (97%)	6 (3%)	40	68
4	D	101/101 (100%)	98 (97%)	3 (3%)	41	69
4	F	101/101 (100%)	97 (96%)	4 (4%)	31	58
All	All	1292/1292 (100%)	1248 (97%)	44 (3%)	37	65

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Н	106	MET
3	L	151	LYS
2	Н	210	LYS
3	3 L		SER
4	F	17	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
4	F	77	ASN
4	4 D		GLN
4	D	13	GLN
2	В	203	ASN
1	A	360	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)

2 ligands 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	Trme	Chain	Dag	Link	Bo	ond leng	ths	В	ond ang	cles			
MIOI	Type	Chain	Chain	Chain	Chain	Res	LIIIK	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	601	1	14,14,15	0.64	0	17,19,21	0.74	1 (5%)			
5	NAG	Е	601	1	14,14,15	0.34	0	17,19,21	0.91	1 (5%)			

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	$\mathbf{Type}$	Chain	$\operatorname{Res}$	Link	Chirals	Torsions	Rings
Ī	5	NAG	A	601	1	-	1/6/23/26	0/1/1/1
	5	NAG	Ε	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

	Mol	Chain	Res	Type	Atoms	Z	$Observed(^o)$	$\operatorname{Ideal}({}^{o})$
	5	Ε	601	NAG	C1-O5-C5	3.35	116.73	112.19
ĺ	5	A	601	NAG	C1-O5-C5	2.25	115.25	112.19

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Ε	601	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	Е	601	NAG	O5-C5-C6-O6
5	A	601	NAG	O5-C5-C6-O6

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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	В	1
2	Н	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	В	132:SER	С	137:GLY	N	7.85
1	Н	132:SER	С	137:GLY	N	6.87



# 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>	$\# \mathrm{RSRZ}{>}2$	$OWAB(A^2)$	Q < 0.9
1	A	197/197 (100%)	0.20	10 (5%) 28 27	27, 51, 127, 207	0
1	E	195/197 (98%)	0.30	7 (3%) 42 42	23, 48, 106, 149	0
2	В	216/216 (100%)	0.16	7 (3%) 47 48	19, 49, 99, 112	0
2	Н	216/216 (100%)	0.26	5 (2%) 60 62	18, 40, 87, 118	0
3	С	219/219 (100%)	0.11	3 (1%) 75 77	26, 50, 79, 106	0
3	L	219/219 (100%)	0.07	1 (0%) 91 92	21, 45, 72, 108	0
4	D	127/127 (100%)	0.08	4 (3%) 49 50	32, 63, 108, 137	0
4	F	127/127 (100%)	0.69	13 (10%) 6 5	37, 65, 97, 154	0
All	All	1516/1518 (99%)	0.21	50 (3%) 46 47	18, 49, 98, 207	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	519	HIS	7.9
1	A	528	LYS	7.7
1	A	333	THR	7.3
1	Е	518	LEU	5.6
1	A	332	ILE	4.9

## 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	$\mathbf{B} ext{-}\mathbf{factors}(\mathbf{\mathring{A}}^2)$	Q<0.9
5	NAG	A	601	14/15	0.92	0.17	57,76,87,91	0
5	NAG	E	601	14/15	0.94	0.20	54,64,68,69	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

