wwPDB X-ray Structure Validation Summary Report (i)

Jun 26, 2024 – 12:18 AM EDT

PDB ID	:	6YM0
Title	:	Crystal structure of the SARS-CoV-2 receptor binding domain in complex with CR3022 Fab (crystal form 1)
Authors	:	Huo, J.; Zhao, Y.; Ren, J.; Zhou, D.; Ginn, H.M.; Fry, E.E.; Owens, R.; Stuart, D.I.
Deposited on	:	2020-04-07
Resolution	:	4.36 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:

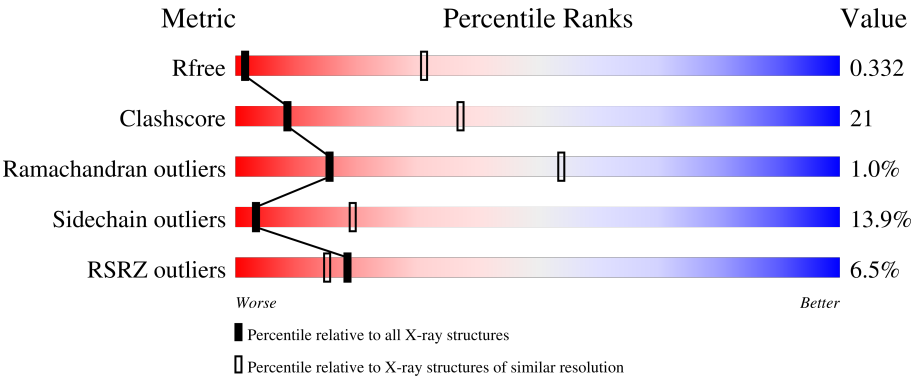
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 4.36 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	1022 (4.92-3.80)
Clashscore	141614	1085 (4.92-3.80)
Ramachandran outliers	138981	1036 (4.92-3.80)
Sidechain outliers	138945	1019 (4.92-3.80)
RSRZ outliers	127900	1091 (5.02-3.70)

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
1	E	213	9%, 55%, 28%, 8%, • 8%
2	H	228	6%, 61%, 27%, 7%, • 5%
3	L	220	3%, 64%, 27%, 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4887 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
			Total	C	N	O	S			
1	E	197	1561	1001	261	291	8	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	327	GLU	-	expression tag	UNP P0DTC2
E	328	THR	-	expression tag	UNP P0DTC2
E	329	GLY	-	expression tag	UNP P0DTC2
E	533	LYS	-	expression tag	UNP P0DTC2
E	534	HIS	-	expression tag	UNP P0DTC2
E	535	HIS	-	expression tag	UNP P0DTC2
E	536	HIS	-	expression tag	UNP P0DTC2
E	537	HIS	-	expression tag	UNP P0DTC2
E	538	HIS	-	expression tag	UNP P0DTC2
E	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	217	1617	1028	263	317	9	0	1	0

- Molecule 3 is a protein called light chain.

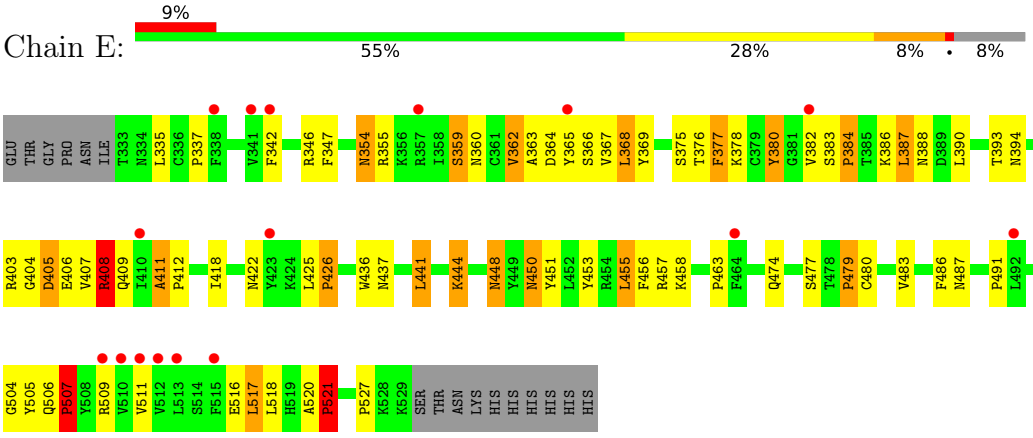
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	220	1709	1073	283	348	5	0	0	0

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.

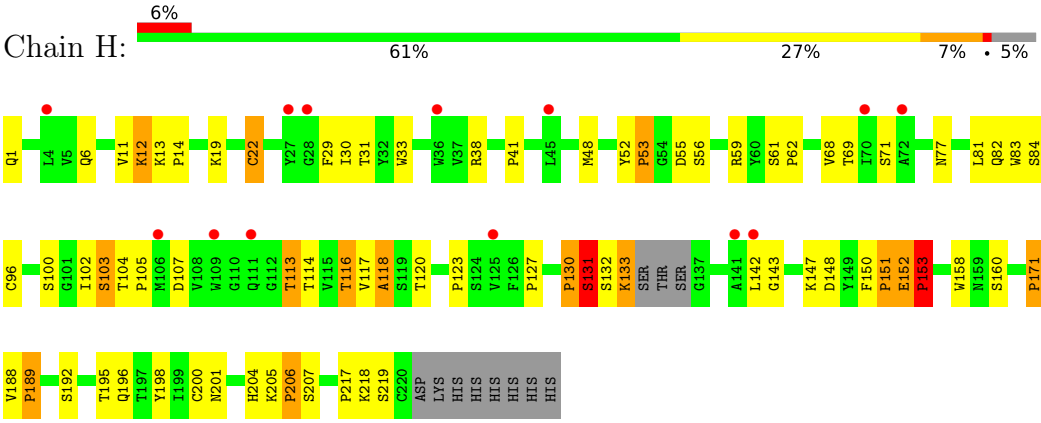
• Molecule 1: Spike glycoprotein

Chain E:



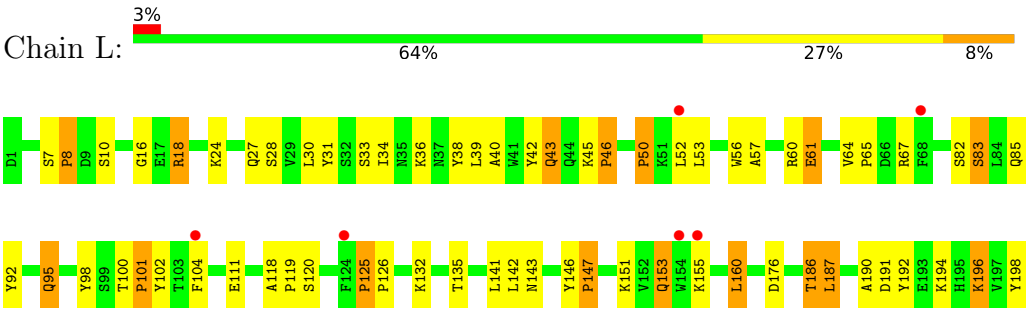
• Molecule 2: heavy chain

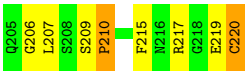
Chain H:



• Molecule 3: light chain

Chain L:




Q205
G206
L207
S208
S209
P210
F215
N216
R217
G218
E219
C220

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	150.47Å 150.47Å 241.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 4.36 79.84 – 4.36	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.00-4.36) 87.9 (79.84-4.36)	Depositor EDS
R_{merge}	0.68	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 4.30Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.323 , 0.319 0.342 , 0.332	Depositor DCC
R_{free} test set	840 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	220.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.20$, $< L^2 > = 0.08$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4887	wwPDB-VP
Average B, all atoms (Å^2)	4.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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

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	E	0.36	3/1605 (0.2%)	0.33	0/2183
2	H	0.43	4/1662 (0.2%)	0.35	0/2262
3	L	0.31	1/1747 (0.1%)	0.28	0/2375
All	All	0.37	8/5014 (0.2%)	0.32	0/6820

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
1	E	0	13
2	H	4	18
3	L	0	11
All	All	4	42

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	210	PRO	N-CD	10.02	1.61	1.47
2	H	153	PRO	N-CD	9.42	1.61	1.47
1	E	507	PRO	N-CD	-7.11	1.37	1.47
1	E	479	PRO	N-CD	-6.84	1.38	1.47
2	H	171	PRO	N-CD	5.96	1.56	1.47

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	131[A]	SER	CA,CA
2	H	131[B]	SER	CA,CA

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	337	PRO	Mainchain
1	E	384	PRO	Mainchain
1	E	408	ARG	Sidechain
1	E	412	PRO	Mainchain
1	E	426	PRO	Mainchain

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	E	1561	0	1486	77	0
2	H	1617	0	1597	65	0
3	L	1709	0	1653	72	0
All	All	4887	0	4736	196	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 21.

The worst 5 of 196 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:E:366:SER:HA	1:E:369:TYR:CE1	1.68	1.28
3:L:146:TYR:CG	3:L:147:PRO:HA	1.79	1.17
2:H:150:PHE:CE1	2:H:151:PRO:HB3	1.79	1.16
2:H:116:THR:HG21	2:H:151:PRO:CG	1.89	1.02
1:E:366:SER:HA	1:E:369:TYR:CZ	1.93	1.02

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	E	195/213 (92%)	178 (91%)	15 (8%)	2 (1%)	15 54
2	H	214/228 (94%)	196 (92%)	16 (8%)	2 (1%)	17 56
3	L	218/220 (99%)	202 (93%)	14 (6%)	2 (1%)	17 56
All	All	627/661 (95%)	576 (92%)	45 (7%)	6 (1%)	15 54

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	118	ALA
2	H	153	PRO
3	L	90	ALA
1	E	521	PRO
1	E	411	ALA

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	E	170/185 (92%)	146 (86%)	24 (14%)	3 19
2	H	183/193 (95%)	156 (85%)	27 (15%)	3 17
3	L	195/195 (100%)	169 (87%)	26 (13%)	4 20
All	All	548/573 (96%)	471 (86%)	77 (14%)	3 19

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	L	43	GLN
3	L	187	LEU
3	L	61	GLU
3	L	132	LYS
3	L	209	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	506	GLN
2	H	3	GLN
3	L	204	HIS
3	L	85	GLN
3	L	95	GLN

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)

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

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	E	197/213 (92%)	0.32	20 (10%) 6 7	4, 4, 4, 4	0
2	H	217/228 (95%)	0.27	14 (6%) 18 15	4, 4, 4, 4	0
3	L	220/220 (100%)	0.11	7 (3%) 47 38	4, 4, 4, 4	0
All	All	634/661 (95%)	0.23	41 (6%) 18 15	4, 4, 4, 4	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	511	VAL	4.6
2	H	111	GLN	4.5
2	H	27	TYR	4.4
1	E	510	VAL	4.1
1	E	410	ILE	4.0

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 (i)

There are no such residues in this entry.