wwPDB X-ray Structure Validation Summary Report (i)

Jun 13, 2024 – 07:34 pm BST

PDB ID	:	8OWV
Title	:	H6 and F2 nanobodies bound to SARS-CoV-2 spike RBD
Authors	:	Mikolajek, H.; Naismith, J.H.; Owens, R.J.
Deposited on	:	2023-04-28
Resolution	:	1.73 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:

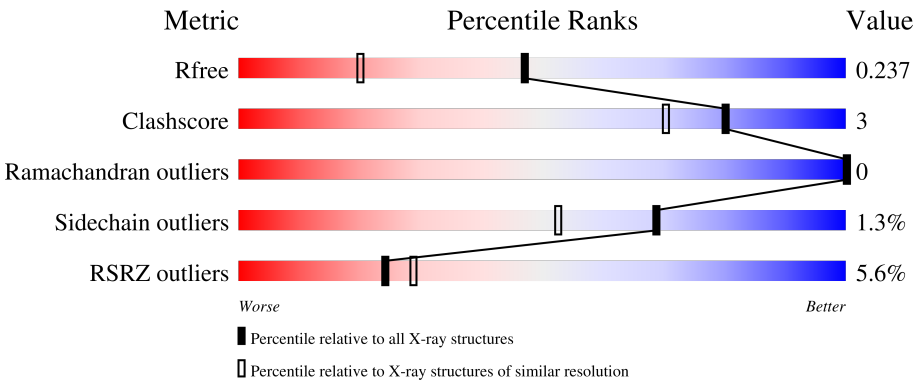
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.73 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	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	EEE	209	3% 90% 5% 5%
2	BBB	132	% 89% 5% • 5%
3	FFF	133	13% 84% 11% 5%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 3782 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 protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	EEE	198	1585	1020	261	296	8	0	4	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EEE	417	VAL	LYS	conflict	UNP P0DTC2
EEE	484	LYS	GLU	variant	UNP P0DTC2
EEE	501	TYR	ASN	variant	UNP P0DTC2
EEE	533	LYS	-	expression tag	UNP P0DTC2
EEE	534	HIS	-	expression tag	UNP P0DTC2
EEE	535	HIS	-	expression tag	UNP P0DTC2
EEE	536	HIS	-	expression tag	UNP P0DTC2
EEE	537	HIS	-	expression tag	UNP P0DTC2
EEE	538	HIS	-	expression tag	UNP P0DTC2
EEE	539	HIS	-	expression tag	UNP P0DTC2

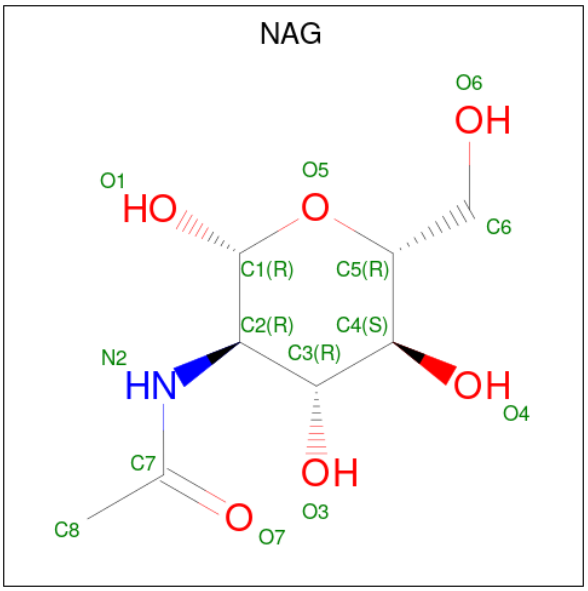
- Molecule 2 is a protein called F2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	BBB	125	987	624	171	188	4	0	0	0

- Molecule 3 is a protein called H6.

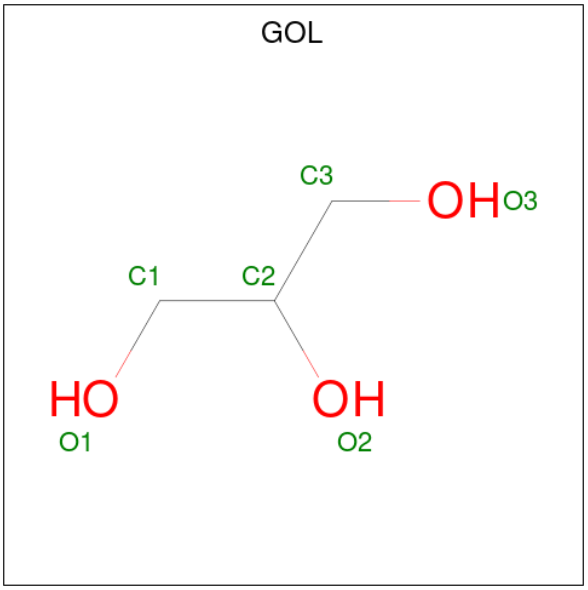
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	FFF	126	962	597	167	192	6	0	2	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	EEE	1	6	3	3		0	0
			Total	C	O			
5	EEE	1	6	3	3		0	0
			Total	C	O			
5	BBB	1	6	3	3		0	0

- Molecule 6 is water.

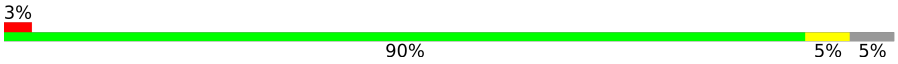
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	EEE	131	131	131	0	0
			Total	O		
6	BBB	61	61	61	0	0
			Total	O		
6	FFF	24	24	24	0	0

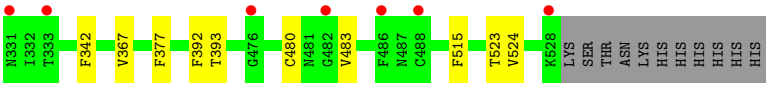
3 Residue-property plots (i)

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 protein S1

Chain EEE:



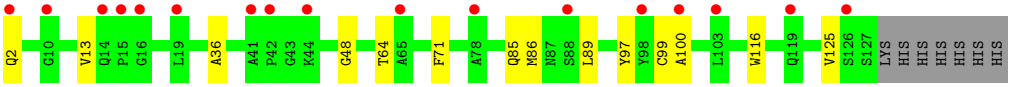


- Molecule 2: F2

Chain BBB:

- Molecule 3: H6

Chain FFF:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	57.77Å 59.44Å 145.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.44 – 1.73 55.03 – 1.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.44-1.73) 100.0 (55.03-1.73)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.223 0.206 , 0.237	Depositor DCC
R_{free} test set	2623 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 37.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3782	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% 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 (i)

5.1 Standard geometry (i)

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

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	EEE	0.64	0/1642	0.78	0/2236
2	BBB	0.64	0/1012	0.81	0/1371
3	FFF	0.67	0/990	0.78	0/1347
All	All	0.65	0/3644	0.79	0/4954

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	EEE	1585	0	1516	6	0
2	BBB	987	0	938	4	0
3	FFF	962	0	920	9	0
4	EEE	14	0	13	2	0
5	BBB	6	0	8	0	0
5	EEE	12	0	16	0	0
6	BBB	61	0	0	1	0
6	EEE	131	0	0	0	0
6	FFF	24	0	0	0	0
All	All	3782	0	3411	19	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 3.

The worst 5 of 19 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:FFF:48:GLY:O	3:FFF:64[B]:THR:HG21	1.87	0.74
1:EEE:523[A]:THR:HG23	1:EEE:524:VAL:HG23	1.70	0.73
2:BBB:102:ARG:NH1	6:BBB:301:HOH:O	2.20	0.72
1:EEE:480:CYS:O	1:EEE:483:VAL:HG22	2.02	0.60
3:FFF:71:PHE:CZ	3:FFF:86:MET:HE2	2.41	0.56

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	EEE	200/209 (96%)	193 (96%)	7 (4%)	0	100	100
2	BBB	123/132 (93%)	119 (97%)	4 (3%)	0	100	100
3	FFF	126/133 (95%)	122 (97%)	4 (3%)	0	100	100
All	All	449/474 (95%)	434 (97%)	15 (3%)	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	EEE	175/182 (96%)	174 (99%)	1 (1%)	86	79
2	BBB	102/109 (94%)	99 (97%)	3 (3%)	42	18
3	FFF	106/111 (96%)	105 (99%)	1 (1%)	78	67
All	All	383/402 (95%)	378 (99%)	5 (1%)	69	52

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	EEE	377	PHE
2	BBB	27	SER
2	BBB	89	LYS
2	BBB	102	ARG
3	FFF	2	GLN

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	EEE	601	1	14,14,15	0.34	0	17,19,21	0.98	0
5	GOL	BBB	201	-	5,5,5	0.11	0	5,5,5	0.33	0
5	GOL	EEE	602	-	5,5,5	0.25	0	5,5,5	0.49	0
5	GOL	EEE	603	-	5,5,5	0.11	0	5,5,5	0.38	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
4	NAG	EEE	601	1	-	0/6/23/26	0/1/1/1
5	GOL	BBB	201	-	-	4/4/4/4	-
5	GOL	EEE	602	-	-	4/4/4/4	-
5	GOL	EEE	603	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	EEE	602	GOL	O1-C1-C2-O2
5	EEE	602	GOL	O1-C1-C2-C3
5	EEE	602	GOL	C1-C2-C3-O3
5	EEE	602	GOL	O2-C2-C3-O3
5	EEE	603	GOL	C1-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	EEE	601	NAG	2	0

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, 95th 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	EEE	198/209 (94%)	0.24	7 (3%) 44 49	20, 32, 59, 87	0
2	BBB	125/132 (94%)	0.25	1 (0%) 86 90	23, 40, 58, 76	0
3	FFF	126/133 (94%)	0.77	17 (13%) 3 4	33, 51, 71, 91	0
All	All	449/474 (94%)	0.39	25 (5%) 24 29	20, 40, 64, 91	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EEE	486	PHE	7.3
1	EEE	331	ASN	5.0
1	EEE	333	THR	4.0
2	BBB	3	GLN	3.6
3	FFF	15	PRO	3.5

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, 95th 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^2)	Q<0.9
5	GOL	EEE	602	6/6	0.79	0.20	28,42,47,53	0
5	GOL	BBB	201	6/6	0.79	0.20	49,63,66,67	0
4	NAG	EEE	601	14/15	0.82	0.18	35,41,44,46	0
5	GOL	EEE	603	6/6	0.87	0.22	37,47,51,66	0

6.5 Other polymers (i)

There are no such residues in this entry.