wwPDB X-ray Structure Validation Summary Report (i)

Aug 7, 2023 – 06:35 PM JST

PDB ID	:	8HR2
Title	:	Ternary Crystal Complex Structure of RBD with NB1B5 and NB1C6
Authors	:	Sun, Z.
Deposited on	:	2022-12-14
Resolution	:	1.94 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:

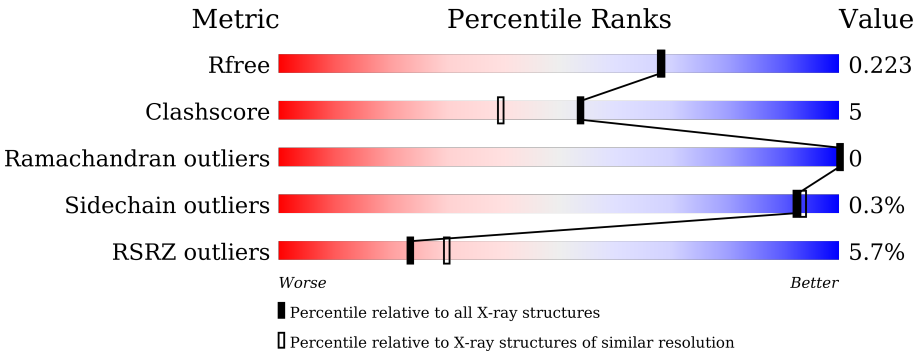
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	A	219	% 73% 11% 15%
2	B	128	2% 94% 5%
3	C	124	16% 77% 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 3592 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
1	A	186	Total	C	N	O	S	0	0	0
			1483	950	246	279	8			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	318	MET	-	expression tag	UNP P0DTC2
A	319	PHE	-	expression tag	UNP P0DTC2
A	320	VAL	-	expression tag	UNP P0DTC2
A	321	PHE	-	expression tag	UNP P0DTC2
A	322	LEU	-	expression tag	UNP P0DTC2
A	323	VAL	-	expression tag	UNP P0DTC2
A	324	LEU	-	expression tag	UNP P0DTC2
A	325	LEU	-	expression tag	UNP P0DTC2
A	326	PRO	-	expression tag	UNP P0DTC2
A	327	LEU	-	expression tag	UNP P0DTC2
A	328	VAL	-	expression tag	UNP P0DTC2
A	329	SER	-	expression tag	UNP P0DTC2
A	330	SER	-	expression tag	UNP P0DTC2
A	331	GLN	-	expression tag	UNP P0DTC2
A	332	CYS	-	expression tag	UNP P0DTC2
A	524	SER	-	expression tag	UNP P0DTC2
A	525	ARG	-	expression tag	UNP P0DTC2
A	526	ALA	-	expression tag	UNP P0DTC2
A	527	ALA	-	expression tag	UNP P0DTC2
A	528	ALA	-	expression tag	UNP P0DTC2
A	529	ASP	-	expression tag	UNP P0DTC2
A	530	TYR	-	expression tag	UNP P0DTC2
A	531	LYS	-	expression tag	UNP P0DTC2
A	532	ASP	-	expression tag	UNP P0DTC2
A	533	ASP	-	expression tag	UNP P0DTC2
A	534	ASP	-	expression tag	UNP P0DTC2
A	535	ASP	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	536	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called NB1C6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	128	Total	C	N	O	S	0	0	0
			981	611	163	199	8			

- Molecule 3 is a protein called NB1B5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	122	Total	C	N	O	S	0	0	0
			938	582	159	191	6			

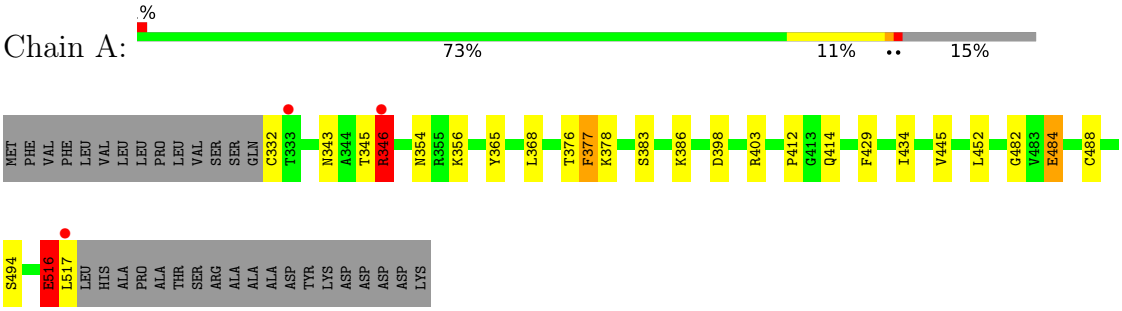
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	109	Total	O	0	0
			109	109		
4	B	65	Total	O	0	0
			65	65		
4	C	16	Total	O	0	0
			16	16		

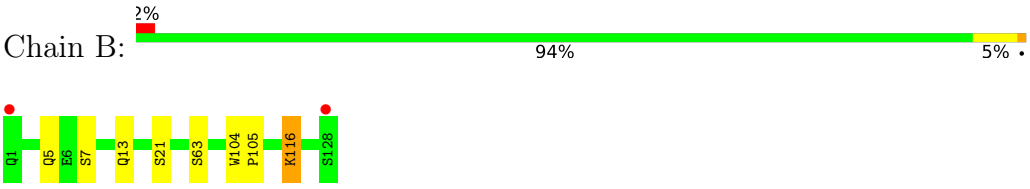
3 Residue-property plots (i)

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.

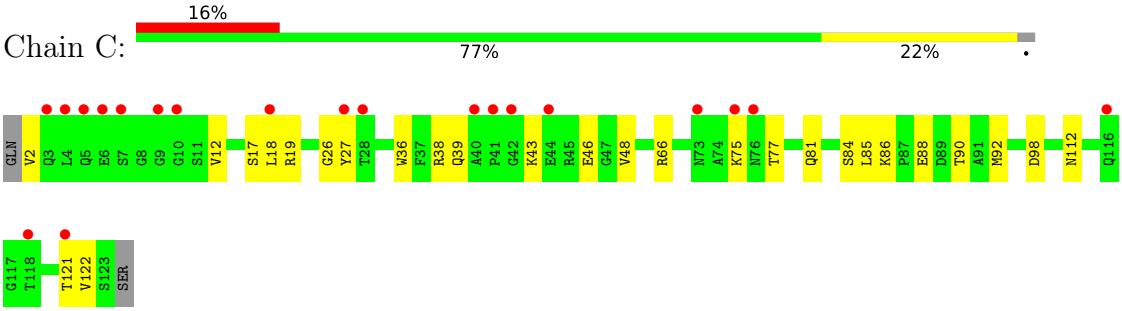
• Molecule 1: Spike protein S1



• Molecule 2: NB1C6



• Molecule 3: NB1B5



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	89.52Å 89.52Å 125.82Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.85 – 1.94 48.85 – 1.94	Depositor EDS
% Data completeness (in resolution range)	89.4 (48.85-1.94) 89.4 (48.85-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 1.94Å)	Xtriage
Refinement program	PHENIX v1.20.1	Depositor
R, R_{free}	0.191 , 0.222 0.191 , 0.223	Depositor DCC
R_{free} test set	1912 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	37.0	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3592	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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	A	0.85	3/1524 (0.2%)	1.36	14/2072 (0.7%)
2	B	0.66	0/1004	0.77	2/1357 (0.1%)
3	C	0.52	0/959	1.46	4/1299 (0.3%)
All	All	0.72	3/3487 (0.1%)	1.25	20/4728 (0.4%)

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	A	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	484	GLU	CD-OE2	12.22	1.39	1.25
1	A	484	GLU	CB-CG	11.01	1.73	1.52
1	A	484	GLU	CG-CD	10.70	1.68	1.51

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	46	GLU	OE1-CD-OE2	-35.39	80.83	123.30
1	A	516	GLU	OE1-CD-OE2	-31.94	84.97	123.30
3	C	46	GLU	CG-CD-OE1	22.06	162.42	118.30
3	C	46	GLU	CG-CD-OE2	-18.26	81.78	118.30
1	A	516	GLU	CG-CD-OE1	18.10	154.49	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	PHE	Sidechain
1	A	516	GLU	Sidechain

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	1483	0	1399	16	0
2	B	981	0	908	5	1
3	C	938	0	868	14	1
4	A	109	0	0	6	0
4	B	65	0	0	1	2
4	C	16	0	0	0	2
All	All	3592	0	3175	35	3

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 5.

The worst 5 of 35 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:A:343:ASN:ND2	4:A:601:HOH:O	1.86	0.91
1:A:414:GLN:NE2	4:A:602:HOH:O	2.02	0.82
2:B:63:SER:O	4:B:201:HOH:O	1.98	0.80
1:A:345:THR:OG1	1:A:346:ARG:NH1	2.20	0.75
3:C:86:LYS:HB3	3:C:88:GLU:OE1	1.89	0.73

All (3) 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-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:GLN:OE1	3:C:84:SER:OG[1_445]	1.70	0.50
4:B:240:HOH:O	4:C:209:HOH:O[1_445]	1.89	0.31
4:B:254:HOH:O	4:C:215:HOH:O[1_445]	2.09	0.11

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	A	184/219 (84%)	176 (96%)	8 (4%)	0	100	100
2	B	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
3	C	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
All	All	430/471 (91%)	418 (97%)	12 (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	A	162/190 (85%)	161 (99%)	1 (1%)	86	85
2	B	100/100 (100%)	100 (100%)	0	100	100
3	C	97/99 (98%)	97 (100%)	0	100	100
All	All	359/389 (92%)	358 (100%)	1 (0%)	92	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	346	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	120	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	186/219 (84%)	0.21	3 (1%) 72 77	26, 41, 62, 75	0
2	B	128/128 (100%)	-0.02	2 (1%) 72 77	25, 40, 63, 84	0
3	C	122/124 (98%)	0.72	20 (16%) 1 2	38, 62, 85, 94	0
All	All	436/471 (92%)	0.28	25 (5%) 23 30	25, 46, 75, 94	0

The worst 5 of 25 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	128	SER	4.8
1	A	333	THR	4.5
3	C	41	PRO	4.2
3	C	44	GLU	4.0
2	B	1	GLN	3.4

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.