

wwPDB X-ray Structure Validation Summary Report (i)

Oct 9, 2023 – 11:42 PM EDT

:	7S7K
:	Crystal structure of the EphB2 extracellular domain
:	Xu, Y.; Xu, K.; Nikolov, D.B.
	2021-09-16
:	3.15 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:

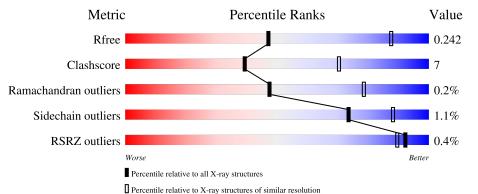
MolProbity	:	4.02b-467
Mogul	:	?.? (???), CSD ??CSD?? (????)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.15 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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	А	525	82%	17%	•
2	В	2	50%	50%	
3	С	3	10	0%	-



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4167 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 Ephrin type-B receptor 2.

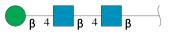
Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	525	Total 4072	C 2543	N 699	O 797	S 33	0	0	0

• Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-a cetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	В	2	Total C N O 28 16 2 10	0	0	0

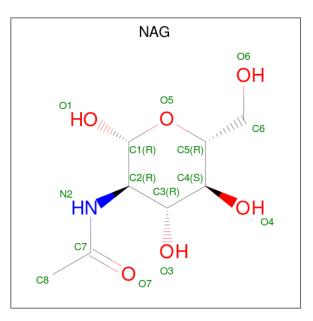
• Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Α	tom	s		ZeroOcc	AltConf	Trace
3	С	3	Total 39	C 22	N 2	0 15	0	0	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
4	А	1	Total C N O 14 8 1 5	0	0
4	А	1	Total C N O 14 8 1 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.

Cl	nai	in	А	: '					_									82	2%														17	7%		-				
V19 E20	E21	127		V37	н36 Р39		0751	D50	T C	OGT	N71		R 80	R85	но <mark>с</mark>	404	T110	N133	P134	A142	1	F147	M157 K158		S165	V169	Y181	1188		Y194	C197	1201	TOOR	ONZT	E215	<mark>\$218</mark>		1227 1227	FO30	
V233	L239	W247	L248	V249	0074	M255	I291		Y310 P311	A311 A312		D315	P316 L317	D318	M319 P320	0701	1324	I332		<mark>5339</mark> L340		E343	P347	L356	N359	1360	I361 C362	K363	C365	R369		Y381	038F	coch	1395	0650	A400	Y404	T405 F406	
E407 1408	0409	V414	T415	0770	0410	F424	N428	I429	T430	1431 N432		S440	0444	* * *	R447	L454	C VE A	070	L471	E475		V495	L498	Y504	R509		T512 V513	A514 C515	Y516	F525	MEOR		L543							

• Molecule 1: Ephrin type-B receptor 2

• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D.		- - • · · · · · · · · · ·
Unam D.	50%	50%

NAG1 NAG2

• Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C:

100%





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants	73.84Å 111.14Å 156.88Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.40 - 3.15	Depositor
Resolution (A)	48.40 - 3.15	EDS
% Data completeness	97.2 (48.40-3.15)	Depositor
(in resolution range)	90.3 (48.40-3.15)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) > 1$	$1.32 (at 3.12 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
D D.	0.214 , 0.248	Depositor
R, R_{free}	0.209 , 0.242	DCC
R_{free} test set	1151 reflections (5.12%)	wwPDB-VP
Wilson B-factor $(Å^2)$	108.3	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 72.4	EDS
L-test for twinning ²	$ \langle L \rangle = 0.48, \langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4167	wwPDB-VP
Average B, all atoms $(Å^2)$	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.33% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities 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: BMA, 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
	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.26	0/4163	0.54	0/5660

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	А	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	133	ASN	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	А	4072	0	3894	60	0
2	В	28	0	25	1	0

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	3	Non-H	1 0	H(added)	Clashes	Symm-Clashes
3	С	39	0	34	0	0
4	А	28	0	26	0	0
All	All	4167	0	3979	60	0

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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 7.

The worst 5 of 60 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:332:ILE:HG23	1:A:343:GLU:HG3	1.59	0.85
1:A:380:GLN:HB2	1:A:396:SER:HB2	1.58	0.85
1:A:332:ILE:HD11	1:A:516:TYR:HE2	1.50	0.75
1:A:495:VAL:HG12	1:A:498:LEU:HD21	1.69	0.75
1:A:206:ILE:HG23	1:A:227:ILE:HG22	1.74	0.70

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	А	523/525~(100%)	502 (96%)	20 (4%)	1 (0%)	47 78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	134	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	А	448/449~(100%)	443~(99%)	5 (1%)	73 88	

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

Mol	Chain	Res	Type
1	А	181	TYR
1	А	315	ASP
1	А	365	CYS
1	А	418	SER
1	А	471	LEU

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

Mol	Chain	Res	Type
1	А	401	HIS

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)

5 monosaccharides are modelled in this entry.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

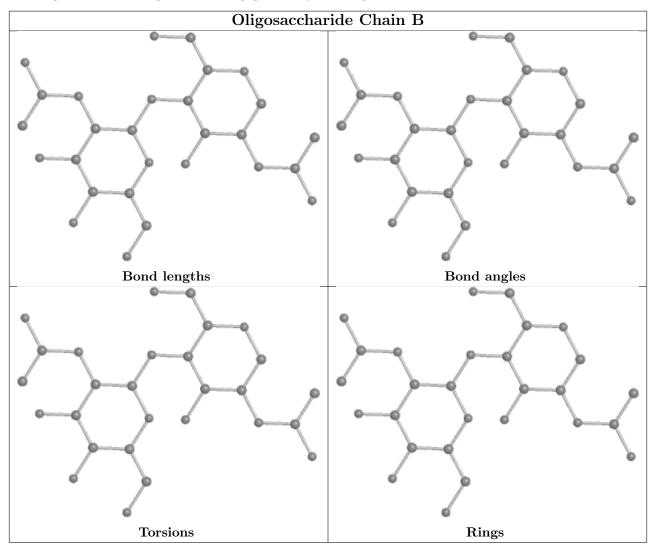


There are no torsion outliers.

There are no ring outliers.

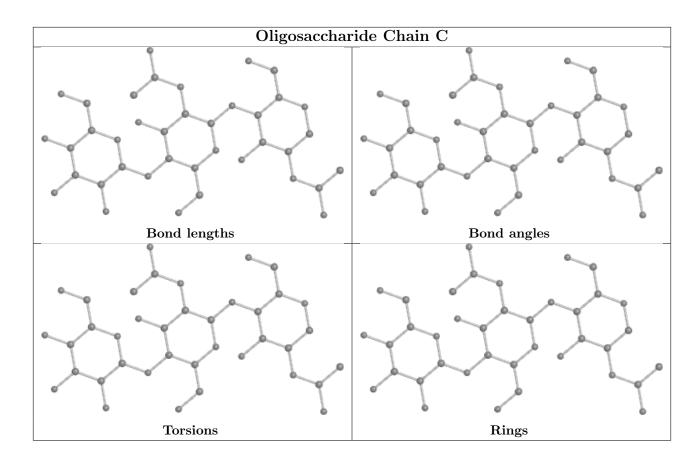
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry (i)

2 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^{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	А	525/525~(100%)	0.03	2 (0%) 92 89	68, 112, 163, 198	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	404	TYR	3.3
1	А	339	SER	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

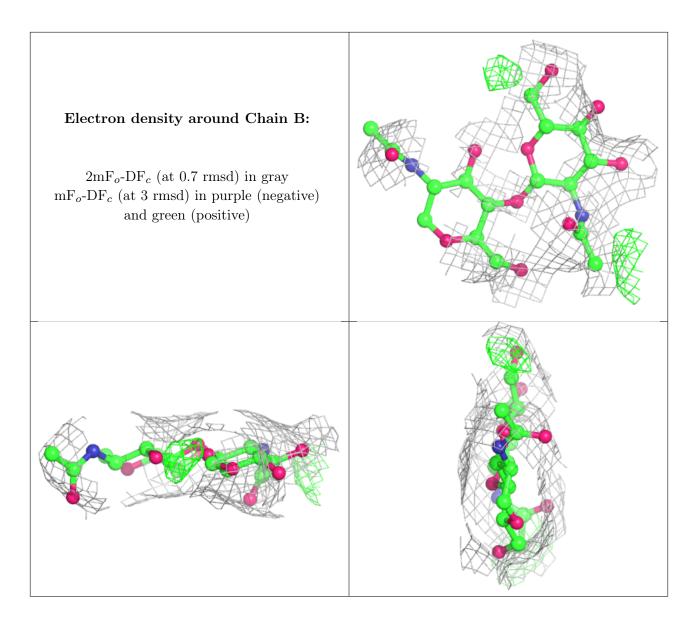
6.3 Carbohydrates (i)

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.

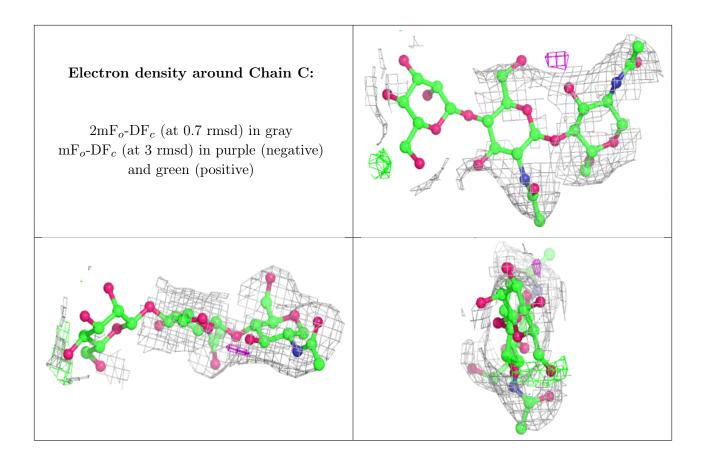
Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(Å^2)$	Q < 0.9
2	NAG	В	2	14/15	0.71	0.27	172,203,216,217	0
3	BMA	С	3	11/12	0.85	0.12	162,175,187,189	0
2	NAG	В	1	14/15	0.88	0.16	146,179,201,211	0
3	NAG	С	1	14/15	0.91	0.16	122,147,158,168	0
3	NAG	С	2	14/15	0.94	0.15	122,163,172,176	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.









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	$B-factors(Å^2)$	Q < 0.9
4	NAG	А	602	14/15	0.77	0.24	138,179,190,191	0
4	NAG	А	601	14/15	0.84	0.15	139,174,185,187	0

6.5 Other polymers (i)

There are no such residues in this entry.

