



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 2, 2025 – 01:59 am GMT

PDB ID : 8RVI
Title : Structure of the binding domain of BoNT/A mutant H1253K in complex with the GM1a ganglioside receptor
Authors : Masuyer, G.; Stenmark, P.
Deposited on : 2024-02-01
Resolution : 1.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

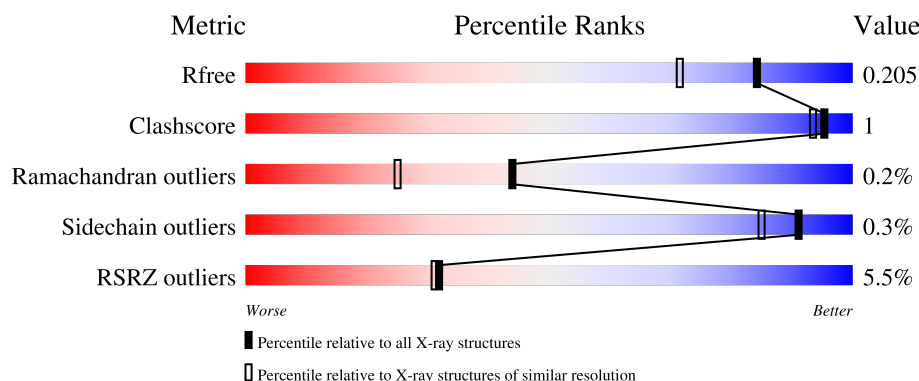
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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 $\leq 5\%$. 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	444	<div> <div>5%</div> <div>90%</div> <div>5%</div> <div>5%</div> </div>
2	G	4	<div> <div>25%</div> <div>75%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3881 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.

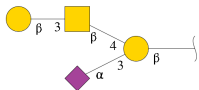
- Molecule 1 is a protein called Botulinum neurotoxin A heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	S	0	4	0
			3475	2214	596	651	14			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	MET	-	initiating methionine	UNP P0DPI0
A	855	GLY	-	expression tag	UNP P0DPI0
A	856	SER	-	expression tag	UNP P0DPI0
A	857	SER	-	expression tag	UNP P0DPI0
A	858	HIS	-	expression tag	UNP P0DPI0
A	859	HIS	-	expression tag	UNP P0DPI0
A	860	HIS	-	expression tag	UNP P0DPI0
A	861	HIS	-	expression tag	UNP P0DPI0
A	862	HIS	-	expression tag	UNP P0DPI0
A	863	HIS	-	expression tag	UNP P0DPI0
A	864	SER	-	expression tag	UNP P0DPI0
A	865	SER	-	expression tag	UNP P0DPI0
A	866	GLY	-	expression tag	UNP P0DPI0
A	867	LEU	-	expression tag	UNP P0DPI0
A	868	VAL	-	expression tag	UNP P0DPI0
A	869	PRO	-	expression tag	UNP P0DPI0
A	870	ARG	-	expression tag	UNP P0DPI0
A	871	GLY	-	expression tag	UNP P0DPI0
A	872	SER	-	expression tag	UNP P0DPI0
A	873	HIS	-	expression tag	UNP P0DPI0
A	874	MET	-	expression tag	UNP P0DPI0
A	875	ASP	-	expression tag	UNP P0DPI0
A	1253	LYS	HIS	engineered mutation	UNP P0DPI0
A	1297	GLN	-	expression tag	UNP P0DPI0

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	4	Total	C	N	O	0	0	0
			56	31	2	23			

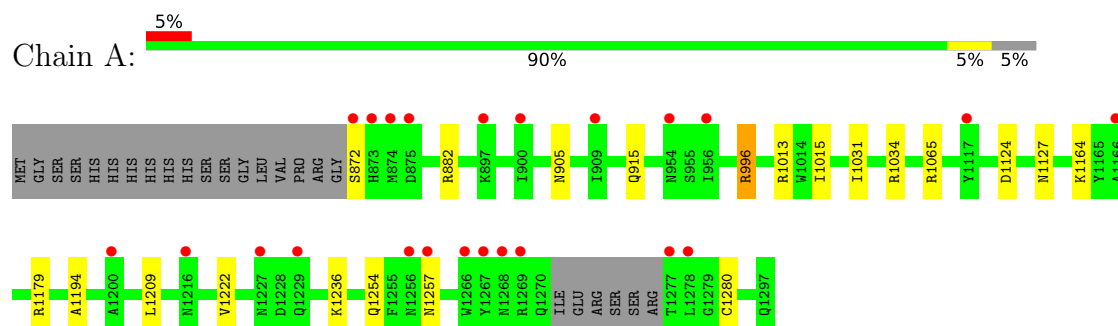
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	350	Total	O	0	0
			350	350		

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: Botulinum neurotoxin A heavy chain



- Molecule 2: beta-D-galactopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-galactopyranose-(1-4)-[N-acetyl-alpha-neuraminic acid-(2-3)]beta-D-galactopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.44Å 114.51Å 106.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.82 – 1.60 61.82 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.82-1.60) 99.8 (61.82-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.172 , 0.197 0.183 , 0.205	Depositor DCC
R_{free} test set	2865 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3881	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SIA, GAL, NGA

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	0.57	0/3555	0.83	7/4805 (0.1%)

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	1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	1034	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	996	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	A	996	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	A	1124	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	1013	ARG	NE-CZ-NH1	5.45	123.02	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	872	SER	Peptide

5.2 Too-close contacts ⓘ

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	3475	0	3432	8	1
2	G	56	0	47	0	0
3	A	350	0	0	2	0
All	All	3881	0	3479	8	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 1.

The worst 5 of 8 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:1236:LYS:NZ	1:A:1280:CYS:SG	2.59	0.76
1:A:1254:GLN:HE21	1:A:1257:ASN:C	2.18	0.46
1:A:996:ARG:HD2	3:A:1343:HOH:O	2.17	0.45
1:A:1164:LYS:NZ	3:A:1305:HOH:O	2.51	0.44
1:A:905[A]:ASN:HB3	1:A:915:GLN:HB3	1.99	0.44

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-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1257:ASN:OD1	1:A:1257:ASN:OD1[3_555]	2.14	0.06

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	420/444 (95%)	404 (96%)	15 (4%)	1 (0%)	44 25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1127	ASN

5.3.2 Protein sidechains ⓘ

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	389/408 (95%)	388 (100%)	1 (0%)	91 85

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

Mol	Chain	Res	Type
1	A	1065	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1026	ASN
1	A	1199	GLN
1	A	1254	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

4 monosaccharides 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
2	GAL	G	1	2	11,11,12	0.52	0	15,15,17	1.07	1 (6%)
2	NGA	G	2	2	14,14,15	0.34	0	17,19,21	0.75	0
2	GAL	G	3	2	11,11,12	0.40	0	15,15,17	0.86	1 (6%)
2	SIA	G	4	2	20,20,21	0.73	0	24,28,31	1.31	3 (12%)

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
2	GAL	G	1	2	-	0/2/19/22	0/1/1/1
2	NGA	G	2	2	-	1/6/23/26	0/1/1/1
2	GAL	G	3	2	-	0/2/19/22	0/1/1/1
2	SIA	G	4	2	-	3/18/34/38	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	4	SIA	C6-O6-C2	3.12	118.01	111.34
2	G	4	SIA	O6-C2-C1	3.03	113.65	107.70
2	G	1	GAL	C1-O5-C5	2.18	115.15	112.19
2	G	3	GAL	O5-C5-C6	2.09	110.48	107.20
2	G	4	SIA	O1B-C1-C2	2.09	118.99	113.03

There are no chirality outliers.

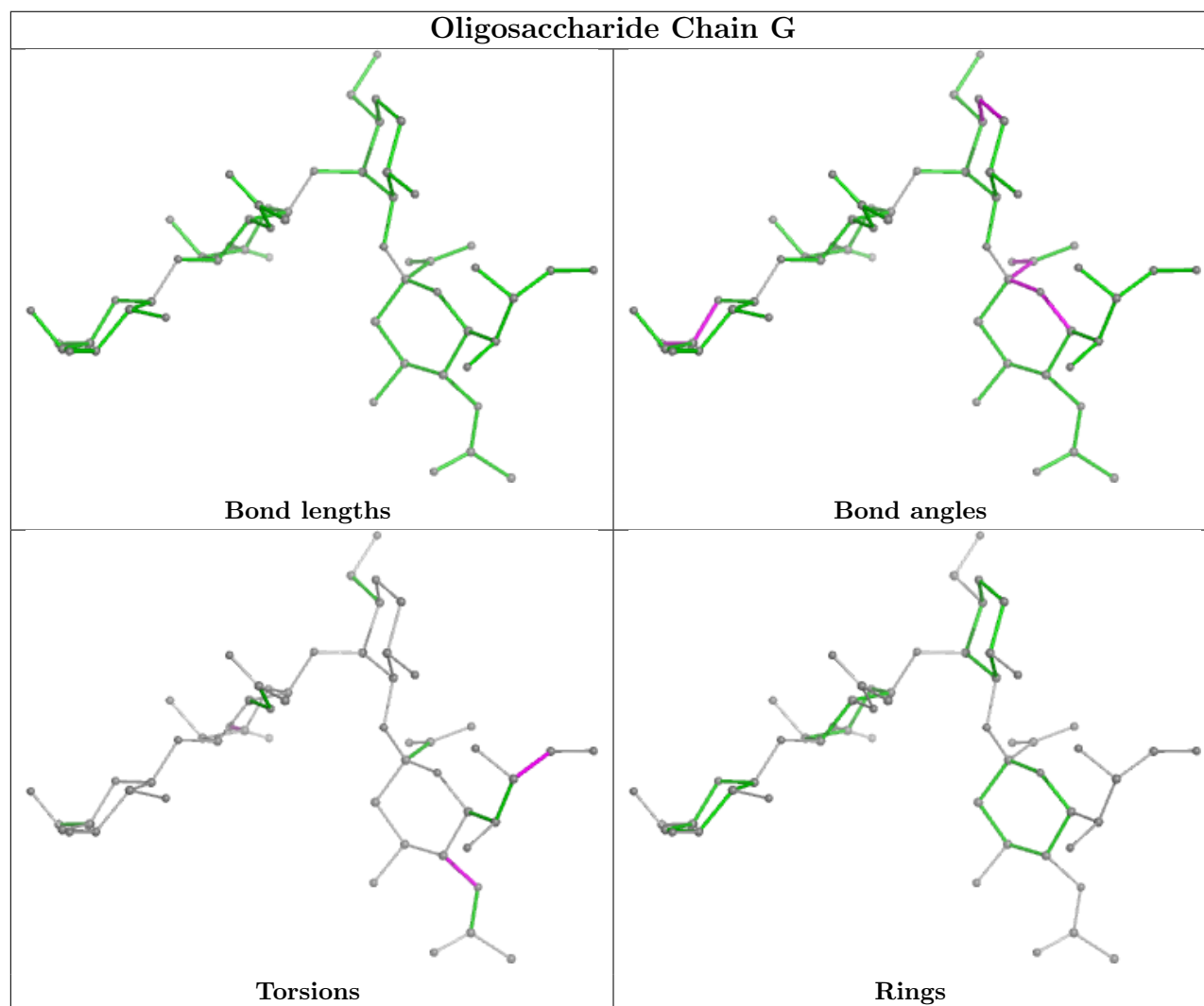
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	4	SIA	O8-C8-C9-O9
2	G	4	SIA	C7-C8-C9-O9
2	G	4	SIA	C4-C5-N5-C10
2	G	2	NGA	C4-C5-C6-O6

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](#)

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 [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	A	420/444 (94%)	0.20	23 (5%)	32 31	14, 25, 44, 69	4 (0%)

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	872	SER	4.6
1	A	1166	ALA	4.2
1	A	1278	LEU	4.1
1	A	873	HIS	3.6
1	A	1266	TRP	3.1

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](#)

SUGAR-RSR INFOmissingINFO

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.