



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 07:36 AM GMT

PDB ID : 2F26
Title : Crystal Structure of the Human Sialidase Neu2 E111Q-Q112E Double Mutant
Authors : Chavas, L.M.G.; Kato, R.; Fusi, P.; Tringali, C.; Venerando, B.; Tettamanti, G.; Monti, E.; Wakatsuki, S.
Deposited on : 2005-11-15
Resolution : 1.58 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

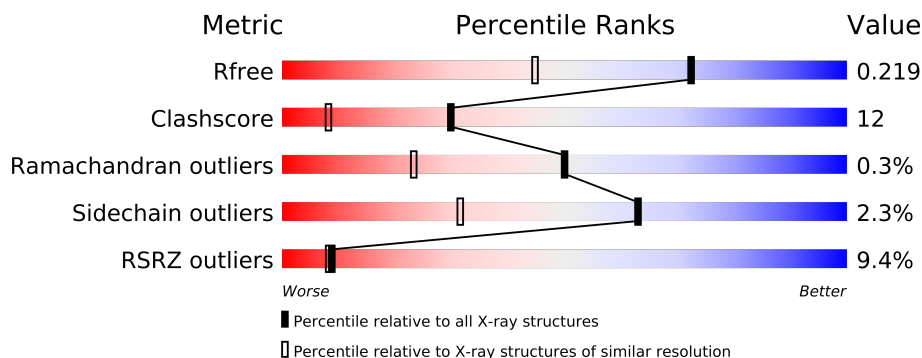
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance


The reported resolution of this entry is 1.58 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}	66092	2778 (1.60-1.56)
Clashscore	79885	3207 (1.60-1.56)
Ramachandran outliers	78287	3107 (1.60-1.56)
Sidechain outliers	78261	3104 (1.60-1.56)
RSRZ outliers	66119	2778 (1.60-1.56)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	382	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3133 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Sialidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	362	2861	1810	510	528	13	0	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	CLONING ARTIFACT	UNP Q9Y3R4
A	0	SER	-	CLONING ARTIFACT	UNP Q9Y3R4
A	111	GLN	GLU	ENGINEERED	UNP Q9Y3R4
A	112	GLU	GLN	ENGINEERED	UNP Q9Y3R4

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

- Molecule 3 is water.

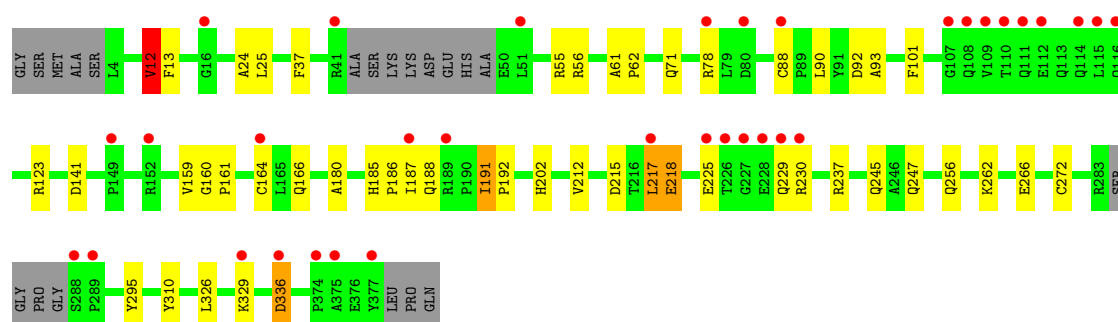
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	271	Total	O	0	0
			271	271		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Sialidase 2

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	145.65Å 145.65Å 64.21Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	72.55 – 1.58 44.99 – 1.58	Depositor EDS
% Data completeness (in resolution range)	99.5 (72.55-1.58) 99.6 (44.99-1.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.61 (at 1.58Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.209 , 0.220 0.208 , 0.219	Depositor DCC
R_{free} test set	3502 reflections (5.06%)	DCC
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 47.2	EDS
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 69226 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3133	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.54	4/2973 (0.1%)	0.82	4/4057 (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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12[A]	VAL	CB-CG1	12.87	1.79	1.52
1	A	12[B]	VAL	CB-CG1	12.87	1.79	1.52
1	A	12[A]	VAL	CB-CG2	-11.23	1.29	1.52
1	A	12[B]	VAL	CB-CG2	-11.23	1.29	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12[A]	VAL	CG1-CB-CG2	20.51	143.71	110.90
1	A	12[B]	VAL	CG1-CB-CG2	20.51	143.71	110.90
1	A	12[A]	VAL	CA-CB-CG1	-11.33	93.91	110.90
1	A	12[B]	VAL	CA-CB-CG1	-11.33	93.91	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	310	TYR	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2861	0	2771	67	0
2	A	1	0	0	0	0
3	A	271	0	0	6	0
All	All	3133	0	2771	67	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (67) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:191:ILE:HD11	1:A:215:ASP:H	1.25	1.01
1:A:12[A]:VAL:CG1	1:A:13:PHE:CD2	2.46	0.98
1:A:88[B]:CYS:HG	1:A:164:CYS:HG	1.07	0.95
1:A:191:ILE:HD11	1:A:215:ASP:N	1.88	0.89
1:A:93:ALA:H	1:A:166:GLN:HE22	1.18	0.88
1:A:326:LEU:HD21	1:A:329:LYS:HG2	1.58	0.85
1:A:185:HIS:HD2	1:A:186:PRO:HD2	1.43	0.82
1:A:217:LEU:HD11	1:A:237:ARG:NE	1.98	0.79
1:A:12[A]:VAL:HG12	1:A:13:PHE:CD2	2.17	0.77
1:A:217:LEU:HD12	1:A:237:ARG:HD3	1.70	0.74
1:A:217:LEU:HG	1:A:237:ARG:HB3	1.70	0.74
1:A:217:LEU:CD1	1:A:237:ARG:CD	2.68	0.71
1:A:247:GLN:HE21	1:A:256:GLN:HE22	1.39	0.70
1:A:247:GLN:HE21	1:A:256:GLN:NE2	1.89	0.69
1:A:217:LEU:HD11	1:A:237:ARG:CD	2.22	0.69
1:A:12[A]:VAL:HG11	1:A:13:PHE:CE2	2.29	0.68
1:A:92:ASP:OD2	1:A:202:HIS:HD2	1.76	0.67
1:A:12[A]:VAL:CG1	1:A:13:PHE:CE2	2.81	0.62
1:A:217:LEU:CD1	1:A:237:ARG:HD3	2.28	0.62
1:A:217:LEU:CD1	1:A:237:ARG:NE	2.63	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:123:ARG:HG2	3:A:1203:HOH:O	2.00	0.61
1:A:185:HIS:CD2	1:A:186:PRO:HD2	2.33	0.60
1:A:123:ARG:HD3	1:A:141:ASP:OD2	2.02	0.59
1:A:12[B]:VAL:CG2	1:A:55:ARG:HD3	2.32	0.59
1:A:12[A]:VAL:CG1	1:A:12[A]:VAL:HB	2.17	0.58
1:A:12[A]:VAL:HG11	1:A:13:PHE:CD2	2.36	0.55
1:A:217:LEU:HD11	1:A:237:ARG:HG2	1.89	0.55
1:A:56:ARG:HG2	3:A:1094:HOH:O	2.06	0.54
1:A:217:LEU:N	1:A:217:LEU:HD23	2.23	0.54
1:A:78:ARG:HG3	3:A:1051:HOH:O	2.09	0.53
1:A:93:ALA:H	1:A:166:GLN:NE2	1.99	0.53
1:A:217:LEU:HD12	1:A:237:ARG:CD	2.36	0.52
1:A:217:LEU:HD11	1:A:237:ARG:CG	2.41	0.50
1:A:187:ILE:HG23	1:A:188:GLN:N	2.27	0.50
1:A:185:HIS:ND1	1:A:188:GLN:HG2	2.27	0.50
1:A:61:ALA:HB3	1:A:62:PRO:HD3	1.94	0.50
1:A:191:ILE:CD1	1:A:215:ASP:H	2.11	0.49
1:A:88[A]:CYS:SG	1:A:160:GLY:HA3	2.53	0.49
1:A:12[B]:VAL:HG22	1:A:55:ARG:HD3	1.94	0.49
1:A:90:LEU:HB2	1:A:164:CYS:HB2	1.95	0.48
1:A:161:PRO:HD2	1:A:218:GLU:HB3	1.95	0.48
1:A:217:LEU:CD1	1:A:237:ARG:CZ	2.92	0.48
1:A:245:GLN:HG2	3:A:1110:HOH:O	2.13	0.47
1:A:237:ARG:HD2	1:A:272:CYS:C	2.35	0.47
1:A:12[A]:VAL:HG12	1:A:13:PHE:N	2.30	0.47
1:A:191:ILE:HD13	1:A:191:ILE:C	2.36	0.46
1:A:55:ARG:HG2	1:A:71:GLN:HA	1.99	0.45
1:A:191:ILE:HD13	1:A:192:PRO:O	2.17	0.45
1:A:217:LEU:HG	1:A:237:ARG:CB	2.44	0.45
1:A:336:ASP:C	1:A:336:ASP:OD2	2.54	0.45
1:A:180:ALA:O	1:A:192:PRO:HA	2.17	0.44
1:A:88[B]:CYS:HB3	1:A:101:PHE:HB2	1.98	0.44
1:A:92:ASP:OD2	1:A:202:HIS:CD2	2.65	0.44
1:A:237:ARG:HA	1:A:266:GLU:OE2	2.17	0.44
1:A:25:LEU:HB3	1:A:336:ASP:OD2	2.18	0.44
1:A:93:ALA:N	1:A:166:GLN:HE22	1.99	0.43
1:A:262:LYS:HG2	3:A:1199:HOH:O	2.19	0.43
1:A:262:LYS:HE3	3:A:1185:HOH:O	2.18	0.43
1:A:24:ALA:HB3	1:A:37:PHE:HB2	2.00	0.43
1:A:88[A]:CYS:SG	1:A:159:VAL:HG23	2.59	0.42
1:A:225:GLU:HG2	1:A:230:ARG:HG2	2.02	0.42

There are no symmetry-related clashes.

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	362/382 (95%)	345 (95%)	16 (4%)	1 (0%)	50 23

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	VAL

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	310/318 (98%)	302 (97%)	8 (3%)	59 26

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12[A]	VAL
1	A	12[B]	VAL
1	A	191	ILE
1	A	217	LEU
1	A	218	GLU
1	A	229	GLN
1	A	295	TYR
1	A	336	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	185	HIS
1	A	202	HIS
1	A	239	HIS
1	A	256	GLN
1	A	259	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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.

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, 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	362/382 (94%)	0.54	34 (9%) 9 8	16, 25, 39, 57	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	227	GLY	13.3
1	A	228	GLU	8.4
1	A	115	LEU	7.0
1	A	217	LEU	7.0
1	A	111	GLN	5.8
1	A	288	SER	5.6
1	A	226	THR	5.5
1	A	229	GLN	4.6
1	A	375	ALA	3.7
1	A	110	THR	3.6
1	A	109	VAL	3.5
1	A	41	ARG	3.5
1	A	225	GLU	3.4
1	A	108	GLN	3.3
1	A	88[A]	CYS	3.3
1	A	116	GLN	3.3
1	A	16	GLY	3.0
1	A	112	GLU	3.0
1	A	78	ARG	3.0
1	A	187	ILE	2.9
1	A	377	TYR	2.9
1	A	114	GLN	2.7
1	A	289	PRO	2.6
1	A	107	GLY	2.6
1	A	152	ARG	2.5
1	A	189	ARG	2.5
1	A	164	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	374	PRO	2.4
1	A	230	ARG	2.4
1	A	329	LYS	2.3
1	A	80	ASP	2.3
1	A	149	PRO	2.3
1	A	51	LEU	2.2
1	A	336	ASP	2.1

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 carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	CL	A	1001	1/1	0.04	-3.15	26,26,26,26	0

6.5 Other polymers ⓘ

There are no such residues in this entry.