



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 22, 2020 – 06:58 AM BST

PDB ID : 1YM4
Title : Crystal structure of human beta secretase complexed with NVP-AMK640
Authors : Hanessian, S.; Yun, H.; Hou, Y.; Yang, G.; Bayrakdarian, M.; Therrien, E.;
Moitessier, N.; Roggo, S.; Veenstra, S.
Deposited on : 2005-01-20
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

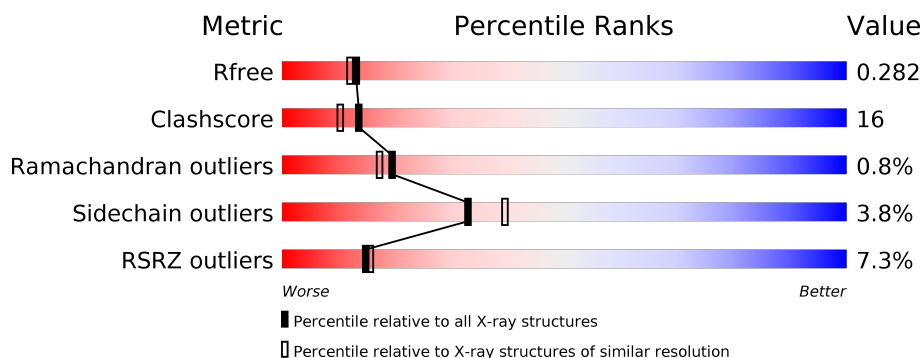
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 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	408	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>19%</div> <div>• 7%</div> </div> </div>
1	B	408	<div> <div>5%</div> <div> <div></div> <div>68%</div> <div>23%</div> <div>• 8%</div> </div> </div>
1	C	408	<div> <div>13%</div> <div> <div></div> <div>52%</div> <div>38%</div> <div>• 7%</div> </div> </div>
2	X	5	<div> <div>20%</div> <div> <div></div> <div>60%</div> <div>20%</div> </div> </div>
2	Y	5	<div> <div>20%</div> <div> <div></div> <div>20%</div> <div>40%</div> <div>20%</div> <div>20%</div> </div> </div>
2	Z	5	<div> <div>20%</div> <div> <div></div> <div>40%</div> <div>40%</div> <div>20%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9538 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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	379	Total	C	N	O	S	0	0	0
			2975	1903	495	563	14			
1	B	377	Total	C	N	O	S	0	0	0
			2966	1898	493	561	14			
1	C	379	Total	C	N	O	S	0	0	0
			2975	1903	495	563	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	GLY	-	EXPRESSION TAG	UNP P56817
A	-14	PRO	-	EXPRESSION TAG	UNP P56817
B	-15	GLY	-	EXPRESSION TAG	UNP P56817
B	-14	PRO	-	EXPRESSION TAG	UNP P56817
C	-15	GLY	-	EXPRESSION TAG	UNP P56817
C	-14	PRO	-	EXPRESSION TAG	UNP P56817

- Molecule 2 is a protein called NVP-AMK640 INHIBITOR.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	X	5	Total	C	N	O	0	0	0
			45	29	6	10			
2	Y	5	Total	C	N	O	0	0	0
			45	29	6	10			
2	Z	5	Total	C	N	O	0	0	0
			45	29	6	10			

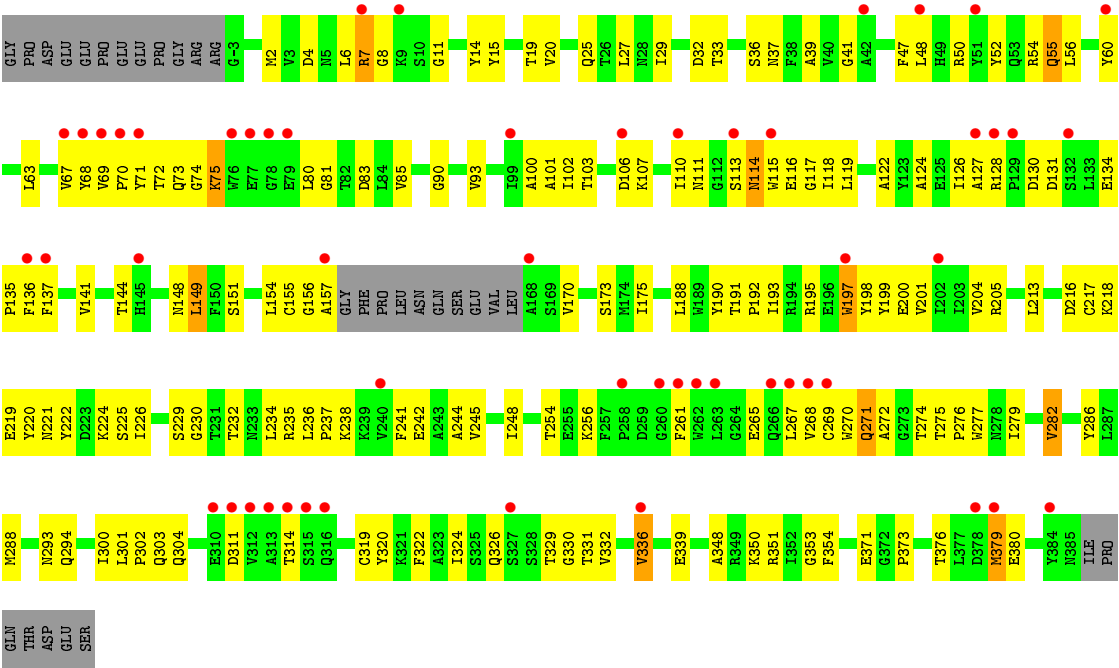
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	203	Total	O	0	0
			203	203		

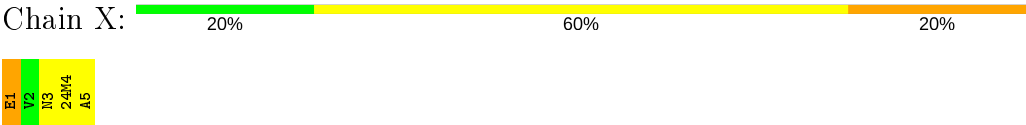
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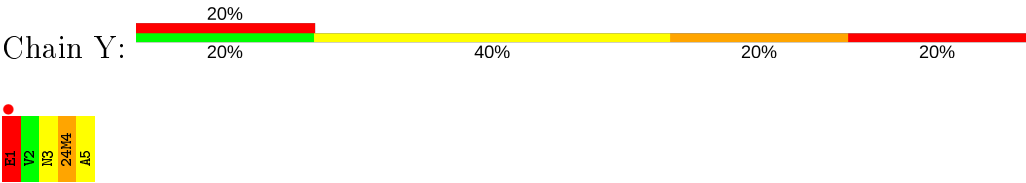
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	155	Total 155	O 155	0	0
3	C	117	Total 117	O 117	0	0
3	X	6	Total 6	O 6	0	0
3	Y	3	Total 3	O 3	0	0
3	Z	3	Total 3	O 3	0	0



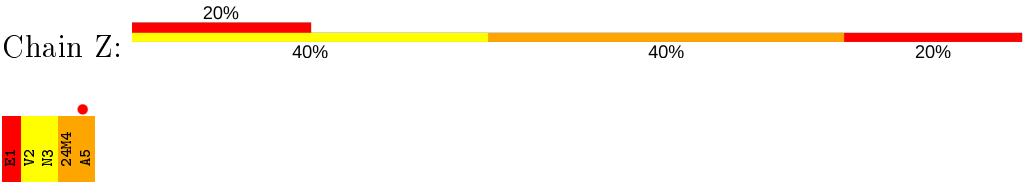
● Molecule 2: NVP-AMK640 INHIBITOR



● Molecule 2: NVP-AMK640 INHIBITOR



● Molecule 2: NVP-AMK640 INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	223.68Å 107.75Å 61.48Å 90.00° 100.32° 90.00°	Depositor
Resolution (Å)	96.77 – 2.25 96.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.3 (96.77-2.25) 99.4 (96.77-2.25)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.25Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.240 , 0.288 0.232 , 0.282	Depositor DCC
R_{free} test set	6850 reflections (10.12%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.741	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9538	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 24M

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	0.45	0/3050	0.69	0/4145
1	B	0.40	0/3041	0.63	1/4133 (0.0%)
1	C	0.37	0/3050	0.58	0/4145
2	X	2.16	2/28 (7.1%)	1.05	0/34
2	Y	2.09	2/28 (7.1%)	0.90	0/34
2	Z	2.36	2/28 (7.1%)	1.03	0/34
All	All	0.46	6/9225 (0.1%)	0.64	1/12525 (0.0%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	1	GLU	CD-OE2	8.95	1.35	1.25
2	X	1	GLU	CD-OE2	8.32	1.34	1.25
2	Y	1	GLU	CD-OE2	8.03	1.34	1.25
2	Z	5	ALA	C-O	6.02	1.34	1.23
2	Y	5	ALA	C-O	5.70	1.34	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	TYR	N-CA-C	-5.64	95.77	111.00

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	A	2975	0	2886	68	0
1	B	2966	0	2878	77	1
1	C	2975	0	2886	145	0
2	X	45	0	47	4	0
2	Y	45	0	47	4	0
2	Z	45	0	47	8	0
3	A	203	0	0	9	0
3	B	155	0	0	14	1
3	C	117	0	0	25	0
3	X	6	0	0	0	0
3	Y	3	0	0	0	0
3	Z	3	0	0	2	0
All	All	9538	0	8791	286	2

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 16.

The worst 5 of 286 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:B:4:ASP:H	1:B:173:SER:HB3	1.32	0.94
1:A:4:ASP:H	1:A:173:SER:HB3	1.31	0.94
1:A:267:LEU:HD22	1:A:309:VAL:HG21	1.49	0.94
1:B:254:THR:HG21	1:B:279:ILE:HB	1.54	0.89
1:B:319:CYS:SG	3:B:2067:HOH:O	2.32	0.87

All (2) 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:B:112:GLY:CA	1:B:112:GLY:CA[2_556]	2.16	0.04
3:B:2152:HOH:O	3:B:2152:HOH:O[2_556]	2.18	0.02

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	375/408 (92%)	349 (93%)	24 (6%)	2 (0%)	29	29
1	B	373/408 (91%)	347 (93%)	24 (6%)	2 (0%)	29	29
1	C	375/408 (92%)	336 (90%)	34 (9%)	5 (1%)	12	8
2	X	1/5 (20%)	1 (100%)	0	0	100	100
2	Y	1/5 (20%)	1 (100%)	0	0	100	100
2	Z	1/5 (20%)	1 (100%)	0	0	100	100
All	All	1126/1239 (91%)	1035 (92%)	82 (7%)	9 (1%)	19	17

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	GLU
1	A	217	CYS
1	B	272	ALA
1	C	80	LEU
1	C	156	GLY

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	322/348 (92%)	313 (97%)	9 (3%)	43	52
1	B	322/348 (92%)	310 (96%)	12 (4%)	34	40
1	C	322/348 (92%)	309 (96%)	13 (4%)	31	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	Y	3/3 (100%)	2 (67%)	1 (33%)	0	0
2	Z	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	975/1053 (93%)	938 (96%)	37 (4%)	33	39

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	197	TRP
1	B	379	MET
2	X	1	GLU
1	B	213	LEU
1	B	282	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	55	GLN
1	B	73	GLN
1	C	271	GLN
1	A	304	GLN
1	C	73	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	24M	Y	4	2	15,15,16	0.78	1 (6%)	12,20,22	1.59	3 (25%)
2	24M	Z	4	2	15,15,16	0.60	0	12,20,22	1.74	4 (33%)
2	24M	X	4	2	15,15,16	0.72	0	12,20,22	1.54	3 (25%)

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	24M	Y	4	2	-	1/13/24/26	0/1/1/1
2	24M	Z	4	2	-	0/13/24/26	0/1/1/1
2	24M	X	4	2	-	1/13/24/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	4	24M	C9-C5	2.01	1.56	1.53

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	4	24M	C19-C9-C11	3.84	107.45	102.76
2	X	4	24M	C39-C36-C3	-3.43	108.44	115.82
2	Y	4	24M	C39-C36-C3	-3.30	108.73	115.82
2	Z	4	24M	C39-C36-C3	-3.11	109.12	115.82
2	Y	4	24M	C19-C9-C11	3.06	106.50	102.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	4	24M	C9-C11-C22-O23
2	Y	4	24M	C9-C11-C22-O23

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	4	24M	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Z	4	24M	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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	379/408 (92%)	0.33	9 (2%) 59 62	22, 36, 65, 104	0
1	B	377/408 (92%)	0.40	20 (5%) 26 29	28, 43, 75, 105	0
1	C	379/408 (92%)	1.00	53 (13%) 2 2	29, 59, 83, 112	0
2	X	4/5 (80%)	0.90	0 100 100	26, 31, 43, 53	0
2	Y	4/5 (80%)	1.43	1 (25%) 0 0	52, 54, 60, 81	0
2	Z	4/5 (80%)	2.35	1 (25%) 0 0	53, 59, 65, 75	0
All	All	1147/1239 (92%)	0.59	84 (7%) 15 15	22, 44, 78, 112	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	112	GLY	7.4
1	C	314	THR	7.4
1	C	312	VAL	5.9
1	B	313	ALA	5.6
1	A	313	ALA	5.6

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	24M	Y	4	15/16	0.90	0.16	45,48,52,54	0
2	24M	Z	4	15/16	0.91	0.18	53,58,65,67	0
2	24M	X	4	15/16	0.94	0.15	24,28,32,32	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.