

wwPDB X-ray Structure Validation Summary Report (i)

Nov 23, 2023 – 02:47 AM JST

PDB ID : 7YU1

Title: Structure of 6-aminohexanoate-oligomer hydrolase NylC precursor,

D122G/H130Y/T267C mutant

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Deposited on : 2022-08-16

Resolution : 1.13 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:

 $Mol Probity \quad : \quad 4.02b\text{--}467$

Mogul: 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13 EDS : 2.36

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $Refmac \quad : \quad 5.8.0158$

CCP4 : 7.0.044 (Gargrove) roteins) : Engh & Huber (2001)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

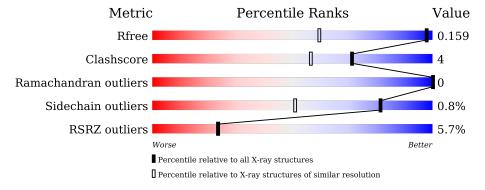
Validation Pipeline (wwPDB-VP) : 2.36

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 1.13 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	Similar resolution
Metric	$(\# \mathrm{Entries})$	$(\# ext{Entries}, ext{ resolution range}(ext{Å}))$
R_{free}	130704	1168 (1.14-1.10)
Clashscore	141614	1205 (1.14-1.10)
Ramachandran outliers	138981	1168 (1.14-1.10)
Sidechain outliers	138945	1165 (1.14-1.10)
RSRZ outliers	127900	1146 (1.14-1.10)

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	355	86%	7%	7%
1	В	355	83%	10%	6%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10738 atoms, of which 4964 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.

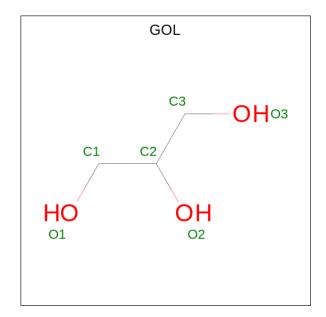
• Molecule 1 is a protein called 6-aminohexanoate-oligomer endohydrolase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace		
1	A	331	Total 4926	C 1560	H 2443	N 439	O 473	S 11	61	8	0
1	В	333	Total 4978	_	H 2473	N 445	O 477	S 10	61	11	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	GLY	ASP	engineered mutation	UNP Q79F77
A	130	TYR	HIS	engineered mutation	UNP Q79F77
Α	267	CYS	THR	engineered mutation	UNP Q79F77
В	122	GLY	ASP	engineered mutation	UNP Q79F77
В	130	TYR	HIS	engineered mutation	UNP Q79F77
В	267	CYS	THR	engineered mutation	UNP Q79F77

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



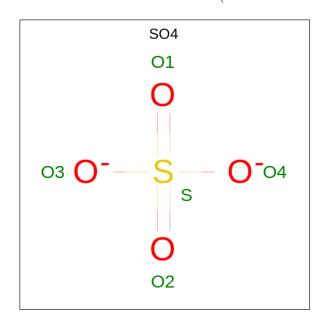


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H O	2	0
			14 3 8 3		_
$\frac{1}{2}$	A	1	Total C H O	2	0
2	Λ	1	14 3 8 3	2	
2	A	1	Total C H O	2	0
2	Λ	1	14 3 8 3	2	
2	A	1	Total C H O	2	0
2	Λ	1	14 3 8 3	2	
2	В	1	Total C H O	2	0
2	Ъ	1	14 3 8 3	2	
2	В	1	Total C H O	2	0
	Б	1	14 3 8 3		

• Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	В	2	Total Na 2 2	0	0

 \bullet Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: $\mathrm{O_4S}).$



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total O S 5 4 1	0	0
4	В	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	В	1	Total O S 5 4 1	0	0

• Molecule 5 is water.

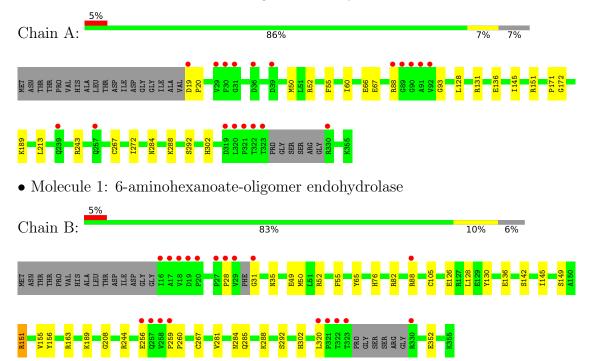
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	374	Total O 374 374	0	0
5	В	358	Total O 358 358	0	0



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.

• Molecule 1: 6-aminohexanoate-oligomer endohydrolase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	69.88Å 144.00Å 129.28Å	Donogitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.27 - 1.13	Depositor
Resolution (A)	28.27 - 1.13	EDS
% Data completeness	98.5 (28.27-1.13)	Depositor
(in resolution range)	87.4 (28.27-1.13)	EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.73 (at 1.13Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
D D	0.129 , 0.155	Depositor
R, R_{free}	0.137 , 0.159	DCC
R_{free} test set	12168 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	11.2	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.44, 55.7	EDS
L-test for twinning ²	$ < L >=0.50, < L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	10738	wwPDB-VP
Average B, all atoms $(Å^2)$	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



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: GOL, NA, SO4

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			nd lengths	Bond angles	
IVIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	A	0.72	$2/2562 \ (0.1\%)$	0.88	2/3481 (0.1%)
1	В	0.75	$2/2588 \; (0.1\%)$	0.94	5/3517 (0.1%)
All	All	0.73	4/5150 (0.1%)	0.91	7/6998 (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
1	В	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\operatorname{Observed}(\text{\AA})$	$\operatorname{Ideal}(ext{\AA})$
1	В	65	TYR	CE2-CZ	5.76	1.46	1.38
1	A	67	GLU	CD-OE2	-5.45	1.19	1.25
1	В	352	GLU	CD-OE1	-5.14	1.20	1.25
1	A	93	GLY	C-O	5.07	1.31	1.23

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

Mol	Chain	Res	Type	Atoms	\mathbf{Z}	$\mathbf{Observed}(^o)$	$Ideal(^{o})$
1	В	244	ARG	NE-CZ-NH2	-10.55	115.03	120.30
1	В	244	ARG	NE-CZ-NH1	8.49	124.54	120.30
1	В	156	TYR	CB-CG-CD1	7.20	125.32	121.00
1	A	243	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	В	156	TYR	CB-CG-CD2	-6.56	117.06	121.00



There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	ARG	Sidechain
1	В	151	ARG	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	2483	2443	2443	11	2
1	В	2505	2473	2474	24	2
2	A	24	32	32	0	0
2	В	12	16	16	0	0
3	A	1	0	0	0	0
3	В	2	0	0	0	0
4	В	15	0	0	3	0
5	A	374	0	0	2	0
5	В	358	0	0	8	0
All	All	5774	4964	4965	35	4

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 4.

The worst 5 of 35 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	$\begin{array}{c} {\rm Interatomic} \\ {\rm distance} ({\rm \AA}) \end{array}$	$egin{aligned} ext{Clash} \ ext{overlap } (ext{Å}) \end{aligned}$	
1:B:28:PRO:HB3	1:B:149:SER:HA	1.73	0.70	
1:A:66:GLU:HG3	5:A:1374:HOH:O	1.97	0.63	
1:B:126:GLU:HG2	1:B:130:TYR:OH	1.99	0.63	
1:A:50[B]:MET:SD	1:A:52:ARG:CZ	2.89	0.60	
1:B:256:GLU:HG3	5:B:649:HOH:O	2.06	0.55	

All (4) 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:292:SER:HG	1:B:302:HIS:HD2[3_857]	1.02	0.58
1:A:292:SER:HG	1:A:302:HIS:HD2[3_857]	1.09	0.51
1:B:88:ARG:HH12	1:B:88:ARG:HH22[3_857]	1.10	0.50
1:A:88:ARG:HH12	1:A:88:ARG:HH22[3_857]	1.21	0.39

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	ysed Favoured Allowed		Outliers	Percentiles		
1	A	336/355~(95%)	324 (96%)	12 (4%)	0	100	100	
1	В	338/355~(95%)	326 (96%)	12 (4%)	0	100	100	
All	All	674/710 (95%)	650 (96%)	24 (4%)	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	252/261 (97%)	250 (99%)	2 (1%)	81 51		
1	В	255/261 (98%)	253 (99%)	2 (1%)	81 51		
All	All	507/522 (97%)	503 (99%)	4 (1%)	81 51		

All (4) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	55	PHE
1	A	189	LYS
1	В	55	PHE
1	В	189	LYS

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	302	HIS
1	В	76	HIS
1	В	302	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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

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			
WIOI	туре	Chain	ites	Lilik	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	В	404	-	4,4,4	0.25	0	6,6,6	0.13	0
2	GOL	В	401	-	5,5,5	0.07	0	5,5,5	0.27	0
2	GOL	В	402	-	5,5,5	0.36	0	5,5,5	0.73	0



Mal	Mol Type	Chain	Res	Link	B	ond leng	$_{ m gths}$	В	ond ang	gles
MIOI	туре	Chain	lites	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	В	403	-	4,4,4	0.39	0	6,6,6	0.19	0
2	GOL	A	1003	-	5,5,5	0.24	0	5,5,5	0.43	0
4	SO4	В	405	_	4,4,4	0.33	0	6,6,6	0.09	0
2	GOL	A	1001	_	5, 5, 5	0.25	0	5,5,5	0.61	0
2	GOL	A	1004	_	5,5,5	0.14	0	5,5,5	0.28	0
2	GOL	A	1002	_	5, 5, 5	0.28	0	5,5,5	0.61	0

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	GOL	В	401	-	-	2/4/4/4	_
2	GOL	В	402	-	-	2/4/4/4	-
2	GOL	A	1003	-	-	2/4/4/4	-
2	GOL	A	1001	-	=	0/4/4/4	-
2	GOL	A	1004	-	-	0/4/4/4	-
2	GOL	A	1002	-	-	2/4/4/4	_

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1002	GOL	C1-C2-C3-O3
2	A	1003	GOL	C1-C2-C3-O3
2	В	401	GOL	C1-C2-C3-O3
2	В	402	GOL	O1-C1-C2-C3
2	A	1003	GOL	O2-C2-C3-O3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	В	404	SO4	1	0
4	В	403	SO4	1	0
4	В	405	SO4	1	0



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	$\langle { m RSRZ} \rangle$	$\#\mathrm{RSRZ}{>}2$		$\mathrm{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	A	331/355 (93%)	0.09	19 (5%) 23	23	10, 15, 30, 56	0
1	В	333/355~(93%)	0.03	19 (5%) 23	23	9, 14, 29, 49	0
All	All	664/710 (93%)	0.06	38 (5%) 23	23	9, 14, 29, 56	0

The worst 5 of 38 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	323	THR	9.5
1	В	323	THR	8.2
1	В	29	VAL	7.4
1	В	322	THR	7.3
1	A	322	THR	6.4

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)

There are no monosaccharides in this entry.

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	$\operatorname{B-factors}(\mathring{\mathrm{A}}^2)$	Q<0.9
4	SO4	В	403	5/5	0.85	0.25	71,83,103,110	0
2	GOL	A	1004	6/6	0.86	0.14	34,47,52,52	2
2	GOL	В	401	6/6	0.91	0.12	27,38,45,50	2
2	GOL	В	402	6/6	0.91	0.20	20,29,38,38	2
2	GOL	A	1001	6/6	0.91	0.16	31,36,49,49	2
2	GOL	A	1002	6/6	0.92	0.15	20,23,26,26	2
4	SO4	В	404	5/5	0.92	0.34	48,56,68,69	0
4	SO4	В	405	5/5	0.93	0.47	54,60,67,72	0
2	GOL	A	1003	6/6	0.94	0.09	21,26,44,50	2
3	NA	A	1005	1/1	0.95	0.51	37,37,37,37	0
3	NA	В	407	1/1	0.98	0.30	30,30,30,30	0
3	NA	В	406	1/1	0.98	0.37	27,27,27,27	0

6.5 Other polymers (i)

There are no such residues in this entry.

