



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 07:20 PM EDT

PDB ID : 6OAZ
Title : Apo Structure of WT Lipoprotein Lipase in Complex with GPIHBP1 Mutant N78D N82D produced in HEK293-F cells
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Deposited on : 2019-03-19
Resolution : 3.04 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : **FAILED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 15843 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 Lipoprotein lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	416	3307	2104	575	612	16	0	0	0
1	B	416	3307	2104	575	612	16	0	0	0
1	C	416	3307	2104	575	612	16	0	0	0
1	D	416	3307	2104	575	612	16	0	0	0

- Molecule 2 is a protein called Glycosylphosphatidylinositol-anchored high density lipoprotein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	83	628	378	110	129	11	0	0	0
2	F	79	594	355	103	125	11	0	0	0
2	G	81	613	367	108	127	11	0	0	0
2	H	80	607	364	107	125	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	78	ASP	ASN	engineered mutation	UNP Q8IV16
E	82	ASP	ASN	engineered mutation	UNP Q8IV16
F	78	ASP	ASN	engineered mutation	UNP Q8IV16
F	82	ASP	ASN	engineered mutation	UNP Q8IV16
G	78	ASP	ASN	engineered mutation	UNP Q8IV16
G	82	ASP	ASN	engineered mutation	UNP Q8IV16
H	78	ASP	ASN	engineered mutation	UNP Q8IV16
H	82	ASP	ASN	engineered mutation	UNP Q8IV16

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Ca 2 2	0	0
5	B	2	Total Ca 2 2	0	0
5	C	2	Total Ca 2 2	0	0
5	D	2	Total Ca 2 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0
6	B	4	Total O 4 4	0	0
6	C	5	Total O 5 5	0	0
6	D	6	Total O 6 6	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	157.00Å 191.94Å 96.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	121.52 – 3.04	Depositor
% Data completeness (in resolution range)	97.0 (121.52-3.04)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 3.01Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.203 , 0.245	Depositor
Wilson B-factor (Å ²)	78.9	Xtrriage
Anisotropy	0.785	Xtrriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	15843	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.6810e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	502	1	14,14,15	0.47	0	17,19,21	1.04	1 (5%)
3	NAG	A	501	1	14,14,15	0.31	0	17,19,21	0.81	1 (5%)
3	NAG	D	502	1	14,14,15	0.40	0	17,19,21	0.95	1 (5%)
4	EDO	C	503	-	3,3,3	0.46	0	2,2,2	0.67	0
4	EDO	A	504	-	3,3,3	0.99	0	2,2,2	0.42	0
4	EDO	D	503	-	3,3,3	1.20	0	2,2,2	0.23	0
3	NAG	A	502	1	14,14,15	0.41	0	17,19,21	1.05	1 (5%)
4	EDO	B	504	-	3,3,3	1.11	0	2,2,2	0.39	0
3	NAG	B	501	1	14,14,15	0.30	0	17,19,21	0.74	1 (5%)
3	NAG	D	501	1	14,14,15	0.31	0	17,19,21	0.79	1 (5%)
4	EDO	D	504	-	3,3,3	1.23	0	2,2,2	0.46	0
4	EDO	A	503	-	3,3,3	0.50	0	2,2,2	0.45	0
4	EDO	C	504	-	3,3,3	1.00	0	2,2,2	0.32	0
3	NAG	C	501	1	14,14,15	0.32	0	17,19,21	0.78	1 (5%)
3	NAG	B	502	1	14,14,15	0.42	0	17,19,21	0.98	1 (5%)
4	EDO	B	503	-	3,3,3	0.55	0	2,2,2	0.62	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
3	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	502	1	-	0/6/23/26	0/1/1/1
4	EDO	C	503	-	-	1/1/1/1	-
4	EDO	A	504	-	-	0/1/1/1	-
4	EDO	D	503	-	-	1/1/1/1	-
3	NAG	A	502	1	-	0/6/23/26	0/1/1/1
4	EDO	B	504	-	-	1/1/1/1	-
3	NAG	B	501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	501	1	-	0/6/23/26	0/1/1/1
4	EDO	D	504	-	-	0/1/1/1	-
4	EDO	A	503	-	-	1/1/1/1	-
4	EDO	C	504	-	-	0/1/1/1	-
3	NAG	C	501	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	502	1	-	0/6/23/26	0/1/1/1
4	EDO	B	503	-	-	1/1/1/1	-

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	NAG	C1-O5-C5	3.92	117.51	112.19
3	C	502	NAG	C1-O5-C5	3.63	117.11	112.19
3	B	502	NAG	C1-O5-C5	3.61	117.09	112.19
3	D	502	NAG	C1-O5-C5	3.26	116.61	112.19
3	A	501	NAG	C1-O5-C5	3.00	116.25	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	EDO	O1-C1-C2-O2
4	C	503	EDO	O1-C1-C2-O2
4	A	503	EDO	O1-C1-C2-O2
4	B	504	EDO	O1-C1-C2-O2
4	D	503	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.